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Patentanmeldung Nr. Patent application No. Demande de brevet n°

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R C van Dijk



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If no title is shown please refer to the description.
Si aucun titre n'est indiqué se référer à la description.)

Crystals of an aurora-a tpx2 complex, tpx2 binding site of aurora-a, aurora-a
ligands and their use

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CRYSTALS OF AN AURORA-A TPX2 COMPLEX, TPX2 BINDING SITE OF AURORA-A, AURORA-A LIGANDS AND THEIR USE

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The present invention relates to crystals of phosphorylated Aurora-A kinase fragment alone
5 and in complex with a ligand, amino acid residues 1-43 of human TPX2. This invention also relates to methods for designing and selecting ligands, in particular allosteric inhibitors of Aurora-A, that bind to the Aurora-A kinase and their use. Further, the present invention relates to certain indene and indole derivatives.

10 At the beginning of mitosis, eukaryotic cells undergo a dramatic reorganization. The nuclear envelope breaks down and microtubules rearrange around chromatin into a bipolar spindle structure that carries out the duty of separating sister chromatids. Chromatin signals to the spindle assembly machinery through Ran, a small Ras-like GTPase that is concentrated in its GTP-bound form around chromatin. Ran function in spindle assembly is connected to its
15 role in nucleocytoplasmic transport. RanGTP releases crucial spindle assembly factors such as TPX2 and NuMA from the transport factors that mediate their import into the nucleus at interphase. After nuclear envelope breakdown, the presence of free TPX2 in the vicinity of chromatin is thought to nucleate microtubules that are subsequently organised into a spindle by microtubule motors. Additionally, TPX2 localises an essential mitotic kinase, Aurora-A, to
20 spindle microtubules (Kufer, T. A., Sillje, H. H., Korner, R., Gruss, O. J., Meraldi, P., and Nigg, E. A. (2002). Human TPX2 is required for targeting Aurora-A kinase to the spindle. *J. Cell Biol.* 158, 617-623).

Aurora kinases constitute a family of serine-threonine protein kinases whose localization and
25 activities are precisely choreographed as a cell progresses through mitosis. Aurora-A is a cell-cycle regulated serine-threonine kinase involved in chromosome segregation and cytokinesis (Bischoff, J.R. and Plowman, G.D. (1999). The Aurora/Ipl1p kinase family: regulators of chromosome segregation and cytokinesis. *Trends Cell Biol.* 9, 454-459). It plays a major role in cell-cycle progression and has also been described as an oncogene. It
30 maps to a chromosome region frequently amplified in tumours (Dutertre, S. et al. (2002). On the role of Aurora A in centrosome function. *Oncogene* 21, 6175-6183). It is overexpressed in a variety of human tumours, in particular breast and colon cancer, but has limited expression in normal tissues (Sen, S. et al. (1997). A putative serine/threonine kinase encoding gene BTAK on chromosome 20q13 is amplified and overexpressed in human
35 breast cancer cell lines. *Oncogene* 14, 2195-2200; Bischoff, J.R. et al. (1998). A homologue of Drosophila Aurora kinase is oncogenic and amplified in human colorectal cancers. *EMBO J.* 17, 3052-3065). Overexpression of active Aurora-A transforms rat fibroblasts so that they

are capable of growing tumours in nude mice, while an inactive mutant is unable to cause oncogenic transformations. As an oncogenic protein kinase, Aurora-A is a target for the development of specific inhibitors that may be useful as cancer therapeutics. Despite the importance of Aurora-A for both cell division and cancer perspectives, little is known at present about its downstream targets and activation/deactivation mechanisms.

Several factors contribute to the activity of a serine/threonine kinase. These include the proper positioning of active site residues and the correct organisation of the substrate-binding site (the "activation segment"). Phosphorylation of a threonine residue within the activation segment is often required to elicit kinase activity and Aurora-A is no exception. Phosphorylation of a threonine in the Aurora-A activation segment (Thr288^{AUR}, human numbering) is crucial for activity, although it is unclear as to whether it is catalysed *in vivo* by an upstream kinase or by Aurora-A itself (Bischoff, et al. (1999) *supra*). Structural studies of c-AMP dependent protein kinase (cAPK) have shown that when the corresponding threonine residue (Thr197^{cAPK}) is phosphorylated, the activation segment is in an active conformation. Cyclin-dependent kinases (CDKs) require not only phosphorylation of the equivalent threonine (Thr160^{CDK}) but also the binding by a partner protein, cyclin-A, to be fully activated. Aurora-A might also rely on a similar mechanism. It has recently been reported that in vertebrates the interaction of Aurora-A with a partner protein, TPX2, leads to a strong activation of the kinase. Upon TPX2 binding, the *in vitro* autophosphorylation activity of Aurora-A is increased and dephosphorylation is prevented (Kufer et al., (2002) *supra*).

ATP competitive inhibitors that are specific for different kinases are used as therapeutic agents in cancer treatment (Garcia-Echeverria, C., et al. (2000). ATP site-directed competitive and irreversible inhibitors of protein kinases. *Med. Res. Rev.* 20, 28-57). Although ATP-binding sites at the moment are the most common targets for the design of kinase inhibitors, it is difficult to achieve selectivity of such inhibitors due to the similarity in kinase active sites, which only have minor differences of surrounding amino-acid residues (Cheetham, G.M.T. et al. (2002). Crystal structure of Aurora-2, an oncogenic serine-threonine kinase. *J. Biol. Chem.* 277, 42419-42422).

The structure of unphosphorylated Aurora-A has been previously reported (Cheetham, G.M.T. et al. (2002). Crystal structure of Aurora-2, an oncogenic serine-threonine kinase. *J. Biol. Chem.* 277, 42419-42422; Nowakowski, J. et al. (2002). Structures of the cancer-related Aurora-A, FAK, and EphA2 protein kinases from nanovolume crystallography. *Structure* 10, 1659-1667). Aurora-A has the typical three-dimensional structure of protein kinases, with the active site situated between the N- and C-terminal lobe. Binding of ATP

involves amino-acid residues that are conserved among all kinases. Extensive structural work has shown that kinases in their active state all assume a similar structural framework, with the 'activation segment' in a similar conformation competent for substrate binding (Huse, M. and Kuriyan, J. (2002). The conformational plasticity of protein kinases. Cell 109, 275-282). However, they differ in the molecular mechanisms to achieve such an active form. In the case of Abl kinase, subtle differences in its activation mechanisms have been exploited with the development of the Abl-specific inhibitor Gleevec, which is used as a leukaemia therapeutic agent (Capdeville, R. et al. (2002). Glivec (STI571, imatinib), a rationally developed, targeted anticancer drug. Nat. Rev. Drug Discov. 1, 493-502).

In the case of Aurora-A, activation is achieved by both phosphorylation and by the binding of a specific activator, the protein TPX2 (Eyers, P.A., et al. (2003). A novel mechanism for activation of the protein kinase Aurora-A. Curr. Biol. 13, 691-697). Blocking this activator-binding site would provide a means to downregulate this kinase specifically.

In view thereof, it was an object of the present invention to elucidate the structure of the Aurora-A TPX2 binding site, to provide means for identifying compounds that bind to Aurora-A and preferably modulate Aurora-A activity, and to provide such compounds.

The present invention relates to (a) crystals of a fragment of phosphorylated human Aurora-A kinase alone (amino acid residues 122-403; hereinafter referred to as Aurora-A(Δ N)), and (b) crystals of said fragment of phosphorylated human Aurora-A kinase in complex with a ligand, i. e. an Aurora-A ligand complex. The Aurora-A ligand is a fragment of TPX2 which is a minimal activating domain of TPX2. The minimal activating domain of TPX2 consists of amino acid residues 1-43 of human TPX2 and hereinafter is referred to as TPX2(1-43).

The present invention provides the structure coordinates of the phosphorylated human Aurora-A(Δ N) kinase. The complete coordinates are listed in Table A.

The present invention also provides the structure coordinates of the phosphorylated human Aurora-A(Δ N)/TPX2(1-43) complex. The complete coordinates are listed in Table B.

The present invention also describes a method for determining at least a portion of the three-dimensional structure of molecules or molecular complexes which contain at least some structurally similar features to the Aurora-A TPX2 binding domain. It is preferred that these molecules or molecular complexes comprise at least a part of the ligand binding site defined by structure coordinates of Aurora-A amino acids Q127, W128, R126, L159, F157,

E170, L169, V206, Y199, H187, R179, L178, V182, Y199, L188, I184, V252, K250, P282, H280 according to Table B, or a mutant or homologue thereof. The numbering system as used herein refers to the protein sequences for human Aurora-A.

- 5 The present invention also provides a machine-readable data storage medium which comprises a data storage material encoded with machine readable data defined by the structure coordinates of phosphorylated human Aurora-A(Δ N) kinase according to Table A or a homologue thereof, or of the phosphorylated human Aurora-A(Δ N)/TPX2(1-43) complex according to Table B.

10

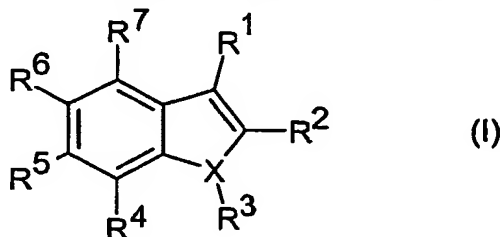
The present invention further provides a binding site in Aurora-A for an Aurora-A ligand such as TPX2 or fragments thereof, as well as methods for designing or selecting further Aurora-A ligands and in particular Aurora-A modulators including agonists, partial agonists, antagonists, partial antagonists of Aurora-A using information about the crystal structures disclosed herein.

15

The present invention further provides allosteric inhibitors of Aurora-A, wherein at least a portion of the inhibitor binds with any portion or all of residues Q127, W128, R126, L159, F157, E170, L169, V206, Y199, H187, R179, L178, V182, Y199, L188, I184, V252, K250, P282, H280 of Aurora-A according to Table B.

20

The present invention in particular relates to indole and indene derivatives of formula (I)



25 wherein

- R¹ represents hydrogen, alkylene-NHR⁸, alkylene-OR⁸, or alkylene-SR⁸;
 R² represents hydrogen, alkylene-NHR⁸, alkylene-OR⁸, or alkylene-SR⁸;
 R³ represents hydrogen, alkyl, alkylene-R⁹, alkenylene-R⁹, alkynylene-R⁹, or arylene-R⁹;
 R⁴ represents hydrogen;
 30 R⁵ represents hydrogen, alkyl, OR¹⁰, NHR¹⁰, SR¹⁰, alkylene-R¹⁰, alkenylene-R¹⁰, alkynylene-R¹⁰, or arylene-R¹⁰;
 R⁶ represents hydrogen, alkyl, OR¹⁰, NHR¹⁰, SR¹⁰, alkylene-R¹⁰, alkenylene-R¹⁰, alkynylene-R¹⁰, or arylene-R¹⁰;

- R^7 represents hydrogen;
 R^8 represents hydrogen, CO-alkyl, $(aa)_m\text{asp}(aa)_n$, $(aa)_m\text{glu}(aa)_n$, or $(aa)_m\text{cys}(aa)_n$;
 R^9 represents NH-alkyl, $N(\text{alkyl})_2$, $N^+(\text{alkyl})_3$, aryl, or heteroaryl;
 R^{10} represents hydrogen, aryl, or substituted aryl;
 5 X represents a nitrogen atom or CH;
 aa represents an amino acid residue; and
 n is zero or an integer of 1 to 10;
 m is zero or an integer of 1 to 10,
 provided that R^1 and R^2 are not both hydrogen and that R^5 and R^6 are not both hydrogen,
 10 and optical isomers, physiologically acceptable salts and prodrugs thereof.

The present invention also relates to the pharmaceutical compositions containing Aurora-A ligands, such as said indole and indene derivatives, and the use of Aurora-A ligands, such as said indole and indene derivatives, in therapy, in particular in cancer treatment.

15

In the drawings the figures show as

- (figure 1) (A) anti-*Xenopus* TPX2 Western blot (upper panel) and anti-*Xenopus* Aurora-A Western blot (lower panel) of GST (glutathione S transferase) (lanes 1 and 2), GST *Xenopus* TPX2 (lanes 3 and 4) or GST *Xenopus* TPX2(1-39) (lanes 5 and 6) which proteins were incubated in *Xenopus* cytosstatic factor (CSF) arrested extracts in the presence or absence of RanQ69L-GTP and immunoprecipitated with GST antibody-coated beads;
 20 (B) anti-GST Western blot (upper panel) and anti-human Aurora-A Western blot (lower panel) of GST (lane 1), GST TPX2(1-43) (lane 2) or GST TPX2(15-43) (lane 3) proteins that were incubated in mitotic HeLa cell extract and immunoprecipitated with GST antibody-coated beads;
 25 (C) autoradiography of the SDS-PAGE gel (left panel) and the corresponding Coomassie-stained gel (right panel) after *in vitro* phosphorylation ($\gamma^{32}\text{P}$ -ATP) of histone H3 by human Aurora-A in the presence of full-length TPX2, GST TPX2(1-43) or GST TPX2(15-43) (lanes 2, 3 and 4 respectively);
 30 (D) much of the phosphorylation signal in GST after *in vitro* phosphorylation ($\gamma^{32}\text{P}$ -ATP) of TPX2(1-43) by Aurora-A (lane 1) followed by TEV cleavage (lane 2);
 35 (E) an anti-human Aurora-A Western blot (upper panel) and an anti-phosphoAurora-A Western blot (lower panel) after phosphatase PP1 treatment of human Aurora-A in the absence or presence of full-length TPX2,

GST TPX2(1-43) or GST TPX2(15-43) followed by detection of Aurora-A by a polyclonal antibody (upper panel) and an antibody specific for Aurora-A phosphorylated at Thr288^{AUR} (lower panel);

(figure 2)

5

(A) an *in vitro* pull-down assay with respect to the binding of full-length Aurora-A, Aurora Δ N or Aurora Δ N(D274N) to GST TPX2(1-43) (lanes 4, 5 and 6), and to GST (lanes 1, 2 and 3);

(B) an anti-phospho Aurora-A Western blot of wild-type Aurora(Δ N) and the D274N mutant when expressed in *E. coli*.

10

(C) autoradiograph for detecting *in vitro* phosphorylation of histone H3 by Aurora(Δ N) in the presence or absense of TPX2(1-43) (lane 2 compared to lane 1), the cleaved (lane 2) or uncleaved (lane 3) GST TPX2(1-43) fusion protein;

15

(D) Sequence alignment of TPX2 N-terminal domain from human (*H*), *Xenopus* (*X*) and puffer fish (*F*), secondary structure elements being shown above the sequences *in red* (upstream extended stretch) and *pink* (downstream helical stretch), and intervening residues not modelled being marked with a dotted line;

20

(E) Sequence alignment of Aurora-A kinase catalytic domain from three vertebrate species that contain TPX2 (human, *H.AUR-A*; *Xenopus*, *X.AUR-A*; puffer fish, *F.AUR-A*), two invertebrates that do not contain TPX2 (*Drosophila*, *D.AUR-A*; *C.elegans*, *C.AUR-A*) together with human and *Xenopus* Aurora-B (*H.AUR-B*, *X.AUR-B*) and vertebrate cAPK, wherein Aurora-A secondary structural elements are labelled above the alignment, the phosphorylated Thr288 (human numbering) is shown, and residues that interact with 7-21^{TPX} or 30-43^{TPX} being indicated by filled or open circles respectively;

25

(figure 3)

ribbon style drawings of the structure of Aurora-A bound to TPX2 as

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(A) a view of the complex between the catalytic domain of human Aurora (Aurora Δ N) and the N-terminal domain of TPX2 shown in typical kinase orientation, an upstream stretch of TPX2 binding at the N-terminal lobe of Aurora-A, and a downstream stretch binding between the two lobes, and a dotted line marking the approximate path of the linker connecting the two TPX2 stretches (disordered and not modelled);

35

(B) a view of the complex after a 180° rotation about the vertical axis in respect to view in panel A showing more clearly the two stretches of TPX2 that bind to Aurora-A;

(C) the upstream stretch of TPX2 (residues 7-21^{TPX}) that binds at a hydrophobic surface groove present in the N-terminal lobe of the kinase,

wherein details of the extensive interactions are shown in the same orientation as in panel B;

(D) the downstream helical stretch of TPX2 (residues 30-43^{TPX}) that binds Aurora-A near helix α C and the activation segment, close to but not directly in contact with phospho-Thr288^{AUR}, wherein details of interactions being shown in the same orientation as in panel B and C.

(figure 4) ribbon style drawings of conformational states of phosphorylated Aurora-A in the presence and absence of TPX2 as

(A) an overlay showing that the structures of Aurora-A when bound to TPX2 and when unbound are closely superposable at the position of active site residues and of helix α C, but diverge at the activation segment between residues His280^{AUR} and Leu293^{AUR}, wherein Phospho-Thr288^{AUR} points inwards in the TPX2-bound structure and outwards in the kinase alone structure;

(B) an illustration of conformational changes upon TPX2 binding, according to which the activation segments of the kinase alone structure (left panel) and of the TPX2-bound structure (right panel) are shown in a view rotated by approximately 90° with respect to panels A-C, and TPX2 binding results in the reorganization of the activation segment, with a 10 Å movement of Thr288^{AUR};

(C) a schematic representation of the molecular mechanism of TPX2-mediated activation of Aurora-A, according to which the upstream stretch of TPX2 anchors the regulator to the N-terminal lobe of the kinase and the downstream stretch (helix) hooks the activation segment triggering a lever-arm like movement, where rotations at His280^{AUR} and Pro282^{AUR} pull on Thr288^{AUR}.

Using X-ray crystallography, crystal structures of phosphorylated human Aurora-A(Δ N) alone at 2.75 Å resolution and in complex with a minimal activating domain of TPX2 at 2.5 Å resolution have been determined and the specific site of TPX2-mediated activation of Aurora-A has been found. TPX2 binds at two sites on the kinase. One stretch of TPX2 (residues 8-19) binds at the N-terminal lobe of the kinase and another stretch (31-38) binds between the two lobes at the phosphorylated activation segment, positioning it for substrate binding. The TPX2-binding site located on the N-terminal lobe of the kinase consists of an extended surface groove formed by Aurora-specific residues. The groove consists of two pockets, one shaped by residues E170, L169, V206, R179, L178, V182, Y199 and the other shaped by residues Q127, W128, R126, L159 and F157. The two pockets are occupied by hydrophobic side chains of TPX2, Y8, Y10, A12 and P13 on one side, and F16, I17 and F19

on the other. From the structure and biochemical data it is concluded that binding of this TPX2 stretch is necessary but not sufficient for activation of Aurora-A, allowing the downstream TPX2 stretch to bind with enough affinity to achieve activation. Binding of a small-molecule inhibitor to the TPX2-recognition groove on the N-terminal lobe of Aurora-A
 5 *would* decrease the activity of this kinase by blocking its specific activation mechanism.

The Aurora-A kinase and the TPX2 protein described herein are intended to include any polypeptide which has the activity of the naturally occurring Aurora-A kinase and TPX2 protein, respectively. Aurora-A and TPX2 contemplated herein include all vertebrate and
 10 mammalian forms such as rat, mouse, pig, goat, horse, guinea pig, rabbit, monkey, orangutan and human. Such terms also include polypeptides that differ from naturally occurring forms of Aurora-A kinase and TPX2 protein by having amino acid deletions, substitutions, and additions, but which retain the activity of Aurora-A kinase and TPX2 protein, respectively. Particular Aurora-A sequences are shown in figure 2E and particular
 15 TPX2 sequences are shown in figure 2D. According to the present invention, the human sequences are preferred.

The crystal structures of the invention preferably contains at least 25%, more preferably at least 50%, more preferably at least 75%, more preferably at least 90%, more preferably at
 20 least 95%, more preferably at least 99%, and most preferably all of the coordinates listed in Table A and Table B, respectively.

The crystal of the phosphorylated human Aurora-A(Δ N) kinase of the invention preferably has the following unit cell dimensions in angstroms: $a = 81.18 \pm 5\%$, $b = 81.18 \pm 5\%$, $c =$
 25 $169.62 \pm 5\%$ and the space group $P6_122$.

The crystal of the phosphorylated human Aurora-A(Δ N) kinase/TPX2(1-43) complex of the invention preferably has the following unit cell dimensions in angstroms: $a = 59.63 \pm 5\%$, $b =$
 30 $81.72 \pm 5\%$, $c = 70.38 \pm 5\%$ and an orthorhombic space group $P2_12_12_1$.

The three-dimensional structure of the phosphorylated human Aurora-A(Δ N) kinase and of the phosphorylated human Aurora-A(Δ N) kinase/TPX2(1-43) complex of this invention are defined by a set of structure coordinates as set forth in Table A and Table B, respectively. The term "structure coordinates" refers to Cartesian coordinates derived from mathematical
 35 equations related to the patterns obtained on diffraction of a monochromatic beam of X-rays by the atoms (scattering centers) of the protein or protein complex in crystal form. The diffraction data are used to calculate an electron density map of the repeating unit of the

crystal. The electron density maps are then used to establish the positions of the individual atoms of the complex.

Those of skill in the art will understand that a set of structure coordinates for a kinase or a kinase/ligand complex or a fragment thereof, is a relative set of points that define a shape in three dimensions. Thus, it is possible that an entirely different set of coordinates could define a similar or identical shape. Moreover, slight variations in the individual coordinates will have little effect on overall shape.

The variations in coordinates discussed above may be generated because of mathematical manipulations of the structure coordinates. For example, the structure coordinates set forth in Table A could be manipulated by crystallographic permutations of the structure coordinates, fractionalization of the structure coordinates; integer additions or subtractions to sets of the structure coordinates, inversion of the structure coordinates or any combination of the above.

Alternatively, modifications in the crystal structure due to mutations, additions, substitutions, and/or deletions of amino acids, or other changes in any of the components that make up the crystal could also account for variations in structure coordinates. If such variations are within an acceptable standard error as compared to the original coordinates, the resulting three-dimensional shape is considered to be the same.

Various computational analyses are therefore necessary to determine whether a molecule or molecular complex or a portion thereof is sufficiently similar to all or parts of the kinase or the kinase/ligand complex described above as to be considered the same. Such analyses may be carried out in current software applications, such as the Molecular Similarity application of QUANTA (Molecular Simulations Inc., San Diego, CA) version 4.1, and as described in the accompanying User's Guide.

The Molecular Similarity application permits comparisons between different structures, different conformations of the same structure, and different parts of the same structure. The procedure used in Molecular Similarity to compare structures is divided into four steps: 1) load the structures to be compared; 2) define the atom equivalences in these structures; 3) perform a fitting operation; and 4) analyze the results.

Each structure is identified by a name. One structure is identified as the target (i. e., the fixed structure); all remaining structures are working structures (i. e., moving structures). Since

atom equivalency within QUANTA is defined by user input, for the purpose of this invention we will define equivalent atoms as protein backbone atoms (N, C and O) for all conserved residues between the two structures being compared. We will also consider only rigid fitting operations.

5

When a rigid fitting method is used, the working structure is translated and rotated to obtain an optimum fit with the target structure. The fitting operation uses an algorithm that computes the optimum translation and rotation to be applied to the moving structure, such that the root mean square difference of the fit over the specified pairs of equivalent atom is an absolute minimum. This number, given in angstroms, is reported by QUANTA.

For the purpose of this invention, any molecule or molecular complex that has a root mean square deviation of conserved residue backbone atoms (N, C, O) of less than 1.5 Å when superimposed on the relevant backbone atoms described by structure coordinates listed in Table A or Table B are considered identical. More preferably, the root mean square deviation is less than 1.0 Å. In a preferred embodiment of the present invention, the molecule or molecular complex comprises at least a portion of the ligand binding site defined by structure coordinates of Aurora-A amino acids Q127, W128, R126, L159, F157, E170, L169, V206, Y199, H187, R179, L178, V182, Y199, L188, I184, V252, K250, P282, H280 according to Table B, or a mutant or homologue of said molecule or molecular complex. More preferred are molecules or molecular complexes comprising all or any part of the ligand binding site defined by structure coordinates of Aurora-A amino acids Y199, L178, W128, H187, L188, I184 according to Table B, or a mutant or homologue of said molecule or molecular complex.

25

The term "complex" or "molecular complex" means Aurora-A or a mutant or homologue of Aurora-A in a covalent or non-covalent association with a chemical entity or compound.

For purposes of the present invention, by "at least a portion of" it is meant all or any part of the ligand binding site defined by these structure coordinates.

By "mutant or homologue" as used herein it is meant a molecule or molecular complex having a similar structure and/or sequences to Aurora-A or TPX2. By "similar structure" it is meant a mutant or homologue having a binding pocket or binding domain that have a root mean square deviation from the backbone atoms of said Aurora-A or TPX2 amino acids of not more than 1.5 Angstroms. By "similar sequence" it is meant a mutant or homologue having 30%, or more preferably 75%, identity with Aurora-A or TPX2 over an amino acid

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sequence of at least 30, preferably at least 50, in particular at least 100 and especially at least 200 consecutive amino acid.

5 The term "root mean square deviation" means the square root of the arithmetic mean of the squares of the deviations from the mean. It is a way to express the deviation or variation from a trend or object. For purposes of this invention, the "root mean square deviation" defines the variation in the backbone of a protein or protein complex from the relevant portion of the backbone of the Aurora-A fragment of the complex as defined by the structure coordinates described herein.

10

Once the structure coordinates of a protein crystal have been determined they are useful in solving the structures of other crystals.

15 Thus, in accordance with the present invention, the structure coordinates of the kinase of the kinase/ligand complex, and portions thereof is stored in a machine-readable storage medium. Such data may be used for a variety of purposes, such as drug discovery and x-ray crystallographic analysis of protein crystals.

20 Accordingly, in one embodiment of this invention is provided a machine-readable data storage medium comprising a data storage material encoded with the structure coordinates set forth in Table A and/or with the structure coordinates set forth in Table B.

25 For the first time, the present invention permits the use of structure-based or rational drug design techniques to design, select, and synthesize chemical entities, including inhibitory and stimulatory compounds that are capable of binding to Aurora-A, or any portion thereof.

30 One particularly useful drug design technique enabled by this invention is iterative drug design. Iterative drug design is a method for optimizing associations between a protein and a compound by determining and evaluating the three-dimensional structures of successive sets of protein/compound complexes.

35 Those of skill in the art will realize that association of natural ligands or substrates with the binding pockets of their corresponding kinases or enzymes is the basis of many biological mechanisms of action. The term "binding pocket" as used herein, refers to a region of a molecule or molecular complex, that, as a result of its shape, favorably associates with another chemical entity or compound. Similarly, many drugs exert their biological effects through association with the binding pockets of kinases and enzymes. Such associations

may occur with all or any parts of the binding pockets. An understanding of such associations will help lead to the design of drugs having more favorable associations with their target kinase, and thus, improved biological effects. Therefore, this information is valuable in designing potential ligands or inhibitors of Aurora-A kinase.

5

The term "associating with" refers to a condition of proximity between chemical entities or compounds, or portions thereof. The association may be non-covalent--wherein the juxtaposition is energetically favored by hydrogen bonding or van der Waals or electrostatic interactions--or it may be covalent.

10

In iterative drug design, crystals of a series of protein/compound complexes are obtained and then the three-dimensional structures of each complex is solved. Such an approach provides insight into the association between the proteins and compounds of each complex. This is accomplished by selecting compounds with inhibitory activity, obtaining crystals of this new protein/compound complex, solving the three-dimensional structure of the complex, and comparing the associations between the new protein/compound complex and previously solved protein/compound complexes. By observing how changes in the compound affected the protein/compound associations, these associations may be optimized.

20

In some cases, iterative drug design is carried out by forming successive protein-compound complexes and then crystallizing each new complex. Alternatively, a pre-formed protein crystal is soaked in the presence of a compound, thereby forming a protein/compound complex and obviating the need to crystallize each individual protein/compound complex.

25

As used herein, the term "soaked" refers to a process in which the crystal is transferred to a solution containing the compound of interest.

The structure coordinates set forth in Table A and Table B can also be used to aid in obtaining structural information about another crystallized molecule or molecular complex.

30

This may be achieved by any of a number of well-known techniques, including molecular replacement.

The structure coordinates set forth in Table A and Table B can also be used for determining at least a portion of the three-dimensional structure of molecules or molecular complexes

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which contain at least some structurally similar features to Aurora-A. In particular, structural information about another crystallized molecule or molecular complex may be obtained. This

may be achieved by any of a number of well-known techniques, including molecular replacement.

Therefore, in another embodiment this invention provides a method of utilizing molecular replacement to obtain structural information about a crystallized molecular complex whose structure is unknown comprising the steps of:

- a) generating an X-ray diffraction pattern from said crystallized molecular complex;
- b) applying at least a portion of the structure coordinates set forth in Table A and Table B to the X-ray diffraction pattern to generate a three-dimensional electron density map of the molecular complex whose structure is unknown; and
- c) using all or a portion of the structure coordinates set forth in Table A and Table B to generate homology models of Aurora-A or any other kinase ligand binding domain.

Preferably, the crystallized molecular complex is obtained by soaking a crystal of this invention in a solution.

By using molecular replacement, all or part of the structure coordinates of the Aurora-A ligand complex provided by this invention or molecular complex whose structure is unknown more quickly and efficiently than attempting to determine such information ab initio.

Molecular replacement provides an accurate estimation of the phases for an unknown structure. Phases are a factor in equations used to solve crystal structures that can not be determined directly. Obtaining accurate values for the phases, by methods other than molecular replacement, is a time-consuming process that involves iterative cycles of approximations and refinements and greatly hinders the solution of crystal structures. However, when the crystal structure of a protein containing at least a homologous portion has been solved, the phases from the known structure provide a satisfactory estimate of the phases for the unknown structure.

Thus, this method involves generating a preliminary model of a molecule or molecular complex whose structure coordinates are unknown, by orienting and positioning the relevant portion of the Aurora-A ligand complex according to Table B within the unit cell of the crystal of the unknown molecule or molecular complex so as best to account for the observed X-ray diffraction pattern of the crystal of the molecule or molecular complex whose structure is unknown. Phases can then be calculated from this model and combined with the observed X-ray diffraction pattern amplitudes to generate an electron density map of the structure whose coordinates are unknown. This, in turn, can be subjected to any well-known model

building and structure refinement techniques to provide a final, accurate structure of the unknown crystallized molecule or molecular complex [E. Lattman, "Use of the Rotation and Translation Functions", in Meth. Enzymol., 115, pp. 55-77 (1985); M. G. Rossmann, ed., "The Molecular Replacement Method", Int. Sci. Rev. Ser., No. 13, Gordon & Breach, New York (1972)].

The structure of any portion of any crystallized molecule or molecular complex, or mutant, or homologue that is sufficiently homologous to any portion of the Aurora-A ligand complex can be solved by this method.

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The structure coordinates are also particularly useful to solve the structure of crystals of Aurora-A ligand co-complexed with a variety of chemical entities. This approach enables the determination of the optimal sites for interaction between chemical entities, including interaction of candidate Aurora-A inhibitors with the complex. For example, high resolution X-ray diffraction data collected from crystals exposed to different types of solvent allows the determination of where each type of solvent molecule resides. Small molecules that bind tightly to these sites can then be designed and synthesized and tested for their Aurora-A inhibition activity.

15

All of the complexes referred to above may be studied using well-known X-ray diffraction techniques and may be refined versus 1.5-3 Å resolution X-ray data to an R value of about 0.20 or less using computer software, such as X-PLOR [Yale University, 1992, distributed by Molecular Simulations, Inc.; see, e. g., Blundell & Johnson, *supra*; Meth. Enzymol., vol. 114 & 115, H. W. Wyckoff et al., eds., Academic Press (1985)]. This information may thus be used to optimize Aurora-A agonists, partial agonists, antagonists, partial antagonists, and more importantly, to design new Aurora-A agonists/antagonists.

25

Accordingly, the present invention is also directed to a binding site in Aurora-A for an Aurora-A ligand in which a portion of Aurora-A ligand is in van der Waals contact or hydrogen bonding contact with at least one of the following residues: Y199, L178, W128, L159, H187, L188, I184 of Aurora-A.

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For purposes of this invention, by Aurora-A binding site it is also meant to include mutants or homologues thereof. In a preferred embodiment, the mutants or homologues have at least 25% identity, more preferably 50% identity, more preferably 75% identity, and most preferably 95% identity to residues Q127, W128, R126, L159, F157, E170, L169, V206,

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Y199, H187, R179, L178, V182, Y199, L188, I184, V252, K250, P282, H280 of Aurora-A binding sites.

The present invention is also directed to a machine-readable data storage medium,
 5 comprising a data storage material encoded with machine readable data, wherein the data is defined by the structure coordinates of an Aurora-A ligand complex according to Table B or a homologue of said complex, wherein said homologue comprises backbone atoms that have a root mean square deviation from the backbone atoms of the complex of not more than 3.0 Å preferably of not more than 2.0 Å.

10

The present invention also provides for computational methods using three-dimensional models of the Aurora-A kinase that are based on crystals of the kinase or the kinase ligand complex. Generally, the computational method of designing an Aurora-A ligand determines which amino acid or amino acids of Aurora-A interact with a chemical moiety (at least one)
 15 of the ligand using a three-dimensional model of a crystallized protein comprising the Aurora-A kinase with a bound ligand and selecting a chemical modification (at least one) of the chemical moiety to produce a second chemical moiety with a structure that either decreases or increases an interaction between the interacting amino acid and the second chemical moiety compared to the interaction between the interacting amino acid and the
 20 corresponding chemical moiety on the natural ligand, i.e. TPX2 or a fragment thereof.

The computational methods of the present invention are for designing kinase synthetic ligands using such crystal and three dimensional structural information to generate synthetic ligands that modulate the conformational changes of the kinase. These computational
 25 methods are particularly useful in designing an agonist, partial agonist, antagonist or partial antagonist to the kinase, wherein the agonist, partial agonist, antagonist or partial antagonist has an extended moiety that prevents any one of a number of ligand-induced molecular events that alter the kinase's influence on one of its targets, such as preventing the normal coordination of the activation domain observed for a naturally occurring ligand or other
 30 ligands that mimic the naturally occurring ligand, such as an agonist. As described herein, synthetic ligands of the kinase will be useful in modulating kinase activity in a variety of medical conditions.

Aurora-A is known to comprise various segments as follows: 1) an amino-terminal ligand-
 35 binding site; and 2) an Aurora-A activation segment.

This modularity permits different segments and sites of each protein to separately accomplish different functions, although the segments and sites influence each other.

- 5 Exploiting the TPX2-binding site in the N-terminal lobe of Aurora-A has the advantage of blocking the activation of this oncogenic kinase and of blocking it specifically. An Aurora-A specific inhibitor would be an important cancer therapeutic agent in particular for breast and colon tumours.

- 10 The polypeptides referred to herein (e. g., Aurora-A, TPX2, and the like) may be produced by any well-known method, including synthetic methods, such as solid phase, liquid phase and combination solid phase/liquid phase syntheses; recombinant DNA methods, including cDNA cloning, optionally combined with site directed mutagenesis; and/or purification of the natural products, optionally combined with enzymatic cleavage methods to produce fragments of naturally occurring forms of Aurora-A and TPX2. The peptides can be
- 15 expressed, crystallized, its three dimensional structure determined with a ligand bound (either using crystal data from the same kinase or a different kinase or a combination thereof), and computational methods used to design ligands to its ligand binding site, particularly ligands that contain an extension moiety that coordinates the activation segment of Aurora-A.

20

Typically Aurora-A and TPX2 as well as fragments thereof are purified to homogeneity for crystallization.

- 25 Purity of Aurora-A is measured with SDS-PAGE, mass spectrometry and hydrophobic HPLC. The purified Aurora-A for crystallization should be at least 97.5 % pure or 97.5%, preferably at least 99.0% pure or 99.0% pure, more preferably at least 99.5% pure or 99.5% pure.

- 30 Initially purification of the unliganded kinase can be obtained by conventional techniques, such as size exclusion chromatography, hydrophobic interaction chromatography (HPLC), ion exchange chromatography (HPLC), and heparin affinity chromatography.

- 35 To achieve higher purification for improved crystals of Aurora-A, it will be desirable to ligand shift purify the kinase using a column that separates the kinase according to charge, such as an ion exchange or hydrophobic interaction column, and then bind the eluted kinase with a ligand, especially an agonist or partial agonist. The ligand induces a change in the kinase's surface charge such that when rechromatographed on the same column, the kinase then

elutes at the position of the liganded kinase are removed by the original column run with the unliganded kinase. Usually saturating concentrations of ligand are used in the column and the protein can be preincubated with the ligand prior to passing it over the column.

- 5 More recently developed methods involve engineering a "tag" such as with histidine placed on the end of the protein, such as on the amino terminus, and then using a nickel chelation column for purification, Janknecht R., Proc. Natl. Acad. Sci. USA Vol 88: 8972-8976 (1991) incorporated by reference.
- 10 Typically, purified Aurora-A is equilibrated at a saturating concentration of ligand at a temperature that preserves the integrity of the protein. Ligand equilibration can be established between 2 and 37 °C, although the kinase tends to be more stable in the 2-20 °C range.

Preferably crystals are made with the hanging and/or sitting drop methods.

15

Regulated temperature control is desirable to improve crystal stability and quality. Temperatures between 4 and 25 °C are generally used and it is often preferable to test crystallization over a range of temperatures. It is preferable to use crystallization temperatures from 18 to 25 °C, more preferably 20 to 23 °C, and most preferably 22 °C.

20

The Aurora-A ligand of this invention is any peptide, peptide mimetic or nonpeptide, including small organic molecules, that is capable of acting as a ligand for Aurora-A. In a preferred embodiment, the Aurora-A ligand is an Aurora-A modulator. By "Aurora-A modulator" it is meant an agonist or activator, a partial agonist or partial activator, an antagonist or inhibitor, or a partial antagonist or partial inhibitor of the Aurora-A kinase.

25

Agonists or partial agonists induce changes in kinases that place them in an active conformation that allows them to influence one of its targets. There may be several different ligand-induced changes in the kinase's conformation.

30

Antagonists or partial antagonists bind to kinases, but fail to induce conformational changes that alter the kinase's target-influencing properties or physiologically relevant conformations. Binding of an antagonist or partial antagonist can also block the binding and therefore the actions of an agonist or partial agonist.

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Partial agonists, or partial antagonists, bind to kinases and induce only part of the changes in the kinases that are induced by agonists or antagonists, respectively. The differences can

be qualitative or quantitative. Thus, a partial agonist or partial antagonist may induce some of the conformation changes induced by agonists or antagonists, respectively, but not others, or it may only induce certain changes to a limited extent.

- 5 As described herein, the unliganded kinase is in a configuration that is either inactive, has some activity or has phosphorylating activity. Binding of agonist ligands induces conformational changes in the kinase such that the kinase becomes more active and/or is protected from deactivation, in particular from dephosphorylation.
- 10 According to a particular embodiment, the present invention relates to allosteric inhibitors of Aurora-A. The binding of such an allosteric inhibitor to Aurora-A results in a conformational change of the kinase, thereby decreasing the kinases's activity, preferably by blocking its activation mechanism. The preferred binding site of an allosteric inhibitor according to the present invention is the TPX2-recognition groove where TPX2 binds Aurora-A, as described
- 15 herein.

Consequently, an extended chemical moiety (or more) from the ligand that stabilizes the binding or contact of the TPX2 binding site with the binding site of Aurora-A can be designed. Typically such chemical moieties will extend past and away from the molecular

20 recognition domain on the ligand and usually past the buried binding cavity of the ligand.

Ligand binding by the kinase is a dynamic process, which regulates kinase function by inducing an altered conformation.

- 25 The three-dimensional structure of the liganded Aurora-A kinase can be used in the development of new Aurora-A synthetic ligands. In addition, Aurora-A is overall well suited to modern methods including three-dimensional structure elucidation and combinatorial chemistry such as those disclosed in EP 335 628, U. S. patent 5,463,564, which are incorporated herein by reference. Computer programs that use crystallography data when
- 30 practicing the present invention enable the rational design of ligands to Aurora-A. Programs such as RASMOL can be used with the atomic coordinates from crystals generated by practicing the invention or used to practice the invention by generating three dimensional models and/or determining the structures involved in ligand binding. Computer programs such as INSIGHT and GRASP allow for further manipulation and the ability to introduce new
- 35 structures. In addition, high throughput binding and bioactivity assays can be devised using purified recombinant protein and modern assays described herein and known in the art in order to refine the structure of a ligand and thereby the activity.

Generally the computational method of designing an Aurora-A synthetic ligand comprises two steps:

- 1) determining which amino acid or amino acids of Aurora-A interacts with a first chemical moiety (at least one) of the ligand using a three dimensional model of a crystallized protein comprising Aurora-A with a bound ligand; and
- 2) selecting chemical modifications (at least one) of the first chemical moiety to produce a second chemical moiety with a structure to either decrease or increase an interaction between the interacting amino acid and the second chemical moiety compared to the interaction between the interacting amino acid and the first chemical moiety.

Preferably the method is carried out wherein said three dimensional model is generated by comparing isomorphous ligand derivatives to produce improved phasing. Further preferred is wherein said method comprises determining a change in interaction between said interacting amino acid and said ligand after chemical modification of said first chemical moiety, especially wherein said three dimensional model is generated by comparing isomorphous ligand derivatives to produce improved phasing. Also preferred is wherein said selecting uses said first chemical moiety that interacts with at least one of the interacting amino acids Y199, L178, W128, L159, H187, L188, I184.

As shown herein, interacting amino acids form contacts with the ligand and the center of the atoms of the interacting amino acids are usually 2 to 4 angstroms away from the center of the atoms of the ligand. Generally these distances are determined by computer, however distances can be determined manually once the three dimensional model is made. See also Wagner et al., Nature 378 (6558): 670-697 (1995) for stereochemical figures of-three dimensional models. More commonly, the atoms of the ligand and the atoms of interacting amino acids are 3 to 4 angstroms apart. The invention can be practiced by repeating steps 1 and 2 to refine the fit of the ligand to the ligand binding site and to determine a better ligand, such as an agonist, partial agonist, antagonist or partial antagonist.

The three dimensional model of Aurora-A can be represented in two dimensions to determine which amino acids contact the ligand and to select a position on the ligand for chemical modification and changing the interaction with a particular amino acid compared to that before chemical modification. The chemical modification may be made using a computer, manually using a two dimensional representation of the three dimensional model or by chemically synthesizing the ligand. The ligand can also interact with distant amino

acids after chemical modification of the ligand to create a new ligand. Distant amino acids are generally not in contact with the ligand before chemical modification. A chemical modification can change the structure of the ligand to make as new ligand that interacts with a distant amino acid usually at least 4.5 angstroms away from the ligand, preferably wherein said first chemical moiety is 6 to 12 angstroms away from a distant amino acid. Often distant amino acids will not line the surface of the binding cavity for the ligand, they are too far away from the ligand to be part of a pocket or binding cavity. The interaction between an amino acid of the ligand binding site and an atom of a ligand can be made by any force or attraction described in nature. Usually the interaction between the atom of the amino acid and the ligand will be the result of a hydrogen bonding interaction, charge interaction, hydrophobic interaction, van der Waals interaction or dipole interaction. In the case of the hydrophobic interaction it is recognized that this is not a per se interaction between the amino acid and ligand, but rather the usual result, in part, of the repulsion of water or other hydrophilic group from a hydrophobic surface. Reducing or enhancing the interaction of the ligand binding site and a ligand can be measured by calculating or testing binding energies, computationally or using thermodynamic or kinetic methods as known in the art.

Chemical modifications will often enhance or reduce interactions of an atom of an amino acid of the ligand binding site and an atom of a ligand. Steric hindrance will be a common means of changing the interaction of the ligand binding cavity with the activation segment.

The present invention also provides methods for identifying compounds that modulate kinase activity. Various methods or combinations thereof can be used to identify these compounds. For example, test compounds can be modeled that fit spatially into the Aurora-A ligand binding site as defined by structure coordinates according to Table B, or using a three-dimensional structural model of Aurora-A, mutant Aurora-A or Aurora-A homolog or portion thereof. Structure coordinates of the ligand binding site, in particular amino acids Q127, W128, R126, L159, F157, E170, L169, V206, Y199, H187, R179, L178, V182, Y199, L188, I184, V252, K250, P282, H280 can also be used to identify structural and chemical features. Identified structural or chemical features can then be employed to design or select compounds as potential Aurora-A modulators. By structural and chemical features it is meant to include, but is not limited to, van der Waals interactions, hydrogen bonding interactions, charge interaction, hydrophobic bonding interaction, hydrophobic interaction and dipole interaction. Alternatively, or in conjunction, the three-dimensional structural model or the ligand binding site can be employed to design or select compounds as potential Aurora-A modulators. Compounds identified as potential Aurora-A modulators can then be

synthesized and screened in an assay characterized by binding of a test compound to the Aurora-A.

Examples of assays useful in screening of potential Aurora-A modulators include, but are not limited to, screening in silico, in vitro assays and high throughput assays, for instance, based on phosphorylation of histone H3 as described herein (Crosio, C., Fimia, G. M., Loury, R., Kimura, M., Okano, Y., Zhou, H., Sen, S., Allis, C. D., and Sassone-Corsi, P. (2002). Mitotic phosphorylation of Histone H3: spatio-temporal regulation by mammalian Aurora kinases. Mol. Cell Biol. 22, 874-885).

A preferred method of the invention can be described as a computational method of designing an kinase antagonist from an kinase agonist comprising:

- 1) determining a structure of a molecular recognition site of said agonist using a three dimensional model of a crystallized protein comprising an Aurora-A, and
- 2) selecting at least one chemical modification of said agonist that provides a ligand structure that extends beyond a binding site for said agonist and in the direction of at least one protein site important in Aurora-A biological function.

Another preferred method of the invention can be described as a computational method of designing a selective kinase modulator such as an kinase super agonist or antagonist comprising:

- 1) determining at least one interacting amino acid of an Aurora-A that interacts with at least one first chemical moiety of said ligand using a three dimensional model of a crystallized protein comprising Aurora-A with a bound ligand, and
- 2) selecting at least one chemical modification of said first chemical moiety to produce a second chemical moiety with a structure to reduce or enhance an interaction between said

interacting amino acid and said second chemical moiety compared to said interaction between said interacting amino acid and said first chemical moiety.

However, as will be understood by those of skill in the art upon this disclosure, other structure based design methods can be used. Various computational structure based design methods have been disclosed in the art.

For example, a number computer modeling systems are available in which the sequence of the Aurora-A and the Aurora-A structure (i. e., atomic coordinates of Aurora-A and/or the atomic coordinates of the active site, the bond and dihedral angles, and distances between

- atoms in the active site such as provided in Table A and Table B) can be input. This computer system then generates the structural details of the site in which a potential Aurora-A modulator binds so that complementary structural details of the potential modulators can be determined. Design in these modeling systems is generally based upon the compound being capable of physically and structurally associating with Aurora-A. In addition, the compound must be able to assume a conformation that allows it to associate with Aurora-A. Some modeling systems estimate the potential inhibitory or binding effect of a potential Aurora-A modulator prior to actual synthesis and testing.
- 10 Methods for screening chemical entities or fragments for their ability to associate with Aurora-A are also well known. Often these methods begin by visual inspection of the active site on the computer screen. Selected fragments or chemical entities are then positioned with the Aurora-A. Docking is accomplished using software such as QUANTA and SYBYL, following by energy minimization and molecular dynamics with standard molecular mechanic
- 15 forcefields such as CHARMM and AMBER. Examples of computer programs which assist in the selection of chemical fragment or chemical entities useful in the present invention include, but are not limited to, GRID (Goodford, P. J. J. Med. Chem. 1985 28: 849-857), AUTODOCK (Goodsell, D. S. and Olsen, A. J. Proteins, Structure, Functions, and Genetics 1990 8: 195-202), and DOCK (Kuntz et al. J. Mol. Biol. 1982 161: 269-288).
- 20 Upon selection of preferred chemical entities or fragments, their relationship to each other and Aurora-A can be visualized and the entities or fragments can be assembled into a single potential modulator.
- 25 Programs useful in assembling the individual chemical entities include, but are not limited to CAVEAT (Bartlett et al. Molecular Recognition in Chemical and Biological Problems Special Publication, Royal Chem. Soc. 78, 182-196 (1989)) and 3D Database systems (Martin, Y. C. J. Med. Chem. 1992 35: 2145-2154).
- 30 Alternatively, compounds may be designed de novo using either an empty active site or optionally including some portion of a known inhibitor. Methods of this type of design include, but are not limited to LUDI (Bohm H-J, J. Comp. Aid. Molec. Design 1992 6: 61-78) and LeapFrog (Tripos Associates, St. Louis. MO).
- 35 Examples of preferred ligands include the above-described indole and indene derivatives of formula (I), and optical isomers, physiologically acceptable salts and prodrugs thereof.

The physiologically acceptable salts in the present case can be acid addition or base addition salts.

For acid addition salts, inorganic acids, such as hydrochloric acid, sulphuric acid, nitric acid or phosphoric acid, or organic acids, in particular carboxylic acids, e.g. acetic acid, tartaric acid, lactic acid, citric acid, malic acid, mandelic acid, ascorbic acid, maleic acid, fumaric acid, gluconic acid or sulphonic acids, e.g. methanesulphonic acid, benzenesulphonic acid and toluenesulphonic acid, and the like are used.

The base addition salts include salts of the compounds of the formula (I) with inorganic bases, such as sodium hydroxide or potassium hydroxide, or with organic bases, such as mono-, di- or triethanolamine.

Prodrugs of the compounds of the formula I are, for example, physiologically easily hydrolysable esters such as alkyl, pivaloyloxymethyl, acetoxymethyl, phthalidyl, indenyl and methoxymethyl esters.

If the compounds according to the invention have asymmetric centres, racemates and optical isomers are included as mixtures or in pure form (enantiomers, diastereomers).

The term "alkyl" includes straight-chain or branched alkyl groups, such as CH_3 , C_2H_5 , n-propyl, $\text{CH}(\text{CH}_3)_2$, n-butyl, $\text{CH}(\text{CH}_3)\text{-C}_2\text{H}_5$, isobutyl, $\text{C}(\text{CH}_3)_3$, n-pentyl or n-hexyl, in particular CH_3 , C_2H_5 or $\text{CH}(\text{CH}_3)_2$, preferably having - if not stated otherwise - 1 to 8, in particular 1 to 6 and particularly preferred 1 to 4 carbon atoms.

The term "alkylene" includes straight-chain or branched alkylene groups, such as methylene and ethylene, preferably having - if not stated otherwise - 1 to 8, in particular 1 to 6 and particularly preferred 1 to 4 carbon atoms.

The term "alkenylene" includes straight-chain or branched, mono- or polyunsaturated alkylene groups, such as ethenylene, preferably having - if not stated otherwise - 2 to 8, in particular 2 to 6 and particularly preferred 2 to 4, carbon atoms.

The term "alkynylene" includes straight-chain or branched, mono- or polyunsaturated alkylene groups, such as ethynylene, preferably having - if not stated otherwise - 2 to 8, in particular 2 to 6 and particularly preferred 2 to 4, carbon atoms.

"Aryl" is in particular a mono- or bicyclic aromatic radical, preferably having 5 to 14 carbon atoms and especially represents naphthyl, indenyl, and in particular phenyl.

"Heteroaryl" is in particular a mono- or bicyclic heteroaromatic radical preferably having 5 to 14 ring atoms and containing 1, 2 or 3 heteroatom(s) independently selected from the group consisting of O, N and S. According to a particular embodiment, bicyclic radicals contain a 5- or 6-membered heteroaromatic radical which is benzo-fused. Heteroaryl includes nitrogen-containing radicals, such as pyrrolyl, imidazolyl, pyrazolyl, pyridazinyl, pyrazinyl, indolyl, quinolinyl, especially pyridyl, pyrimidyl and isoquinolinyl; radicals which contain an oxygen atom or a sulphur atom, such as thienyl, benzothienyl, furanyl and especially benzofuranyl; radicals which contain two or more different heteroatoms, such as thiazolyl, isothiazolyl, thiadiazolyl, isoxazolyl and oxazolyl. Preferred aromatic heterocyclic radicals are, pyridyl and indolyl.

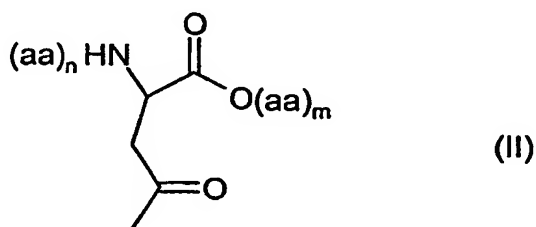
The term "arylene" is preferably naphthylene and in particular phenylene, such as 1,4-phenylene.

According to a preferred embodiment, one of residues R^1 and R^2 , preferably residue R^2 , is hydrogen while the other, preferably R^1 , has a meaning different from hydrogen. In this context, alkylene radicals preferably contain a relatively short main chain connecting the indole or indene moiety with the amino, oxy or thio moiety ($-NHR^8$, $-OR^8$ or $-SR^8$, respectively). Accordingly, the main chain of preferred alkylene radicals contain 1 to 3 carbon atoms. Said alkylene radicals may be branched. Linear alkylene radicals are preferred. Specific examples of alkylene radicals include methylene, eth-1,1-ylene, prop-1,1-ylene and prop-2,2-ylene, with methylene being preferred.

According to a particularly preferred embodiment, one of residues R^1 and R^2 , preferably R^2 , is hydrogen and the other, preferably R^1 , represents alkylene- NHR^8 .

R^8 preferably represents an acyl radical so as to form an amide, ester or thioester bond within residue R^1 and/or R^2 . It is preferred that residue R^8 represents an amino acid selected from the group consisting of aspartate (asp), glutamate (glu), and cysteine (cys), i.e., n and m are zero, or a peptide connected via aspartate, glutamate or cysteine, i.e., aa represents an amino acid radical, and at least one of n and m is an integer of 1 or higher, wherein the amino acid radicals can be the same or different. The aspartate, glutamate and cysteine radicals may be bonded to the alkylene radical via any of their functional groups. The aspartate and glutamate radicals are preferably bonded via any of its carboxy groups, the β -

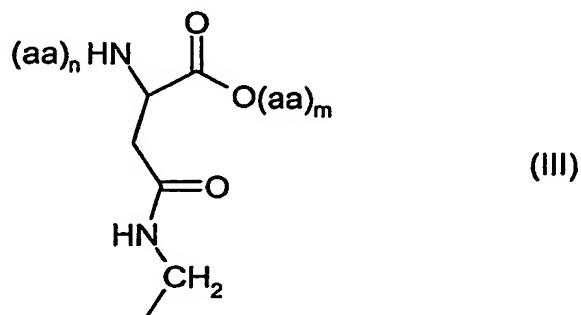
carboxy function of aspartate and the γ -carboxy function of glutamate being preferred. Cystein radicals are preferably bonded via their side chain thio functionality. Accordingly, the amino acid radicals aa are connected to the alkylene group via the remaining functional groups of the aspartate, glutamate or cysteine radicals. According to a preferred embodiment, the remaining functional groups are the α -amino group and the α -carboxy group, of which one or both can be bonded to the amino acid radicals aa. According to this embodiment, the connecting aspartate, glutamate or cystein radical is itself part of the peptide chain which is connected to the alkylene residue via the side chain of said aspartate, glutamate or cystein radical. A specific example of such a preferred residue R⁸ is a radical of the formula (II)



wherein

- aa represents an amino acid radical;
 n is zero or an integer of 1 to 10; and
 m is zero or an integer of 1 to 10.

A specific example of such preferred residues R1 and/or R2 is thus the radical of formula (III)



wherein

- aa represents an amino acid radical;
 n is zero or an integer of 1 to 10; and
 m is zero or an integer of 1 to 10.

The amino acid radicals aa may be any amino acid. Preferably said amino acid radicals are selected to mimic – together with the connecting amino acid – a portion of TPX2 that binds to Aurora-A. Said portion of TPX2 is in particular a portion comprising the amino acid

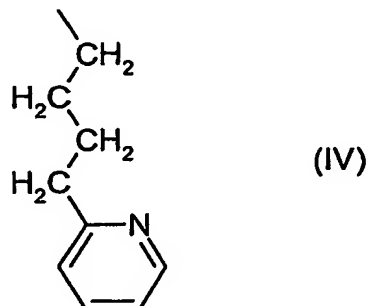
sequence from residues 7 to 21, preferably 8 to 19 (compare Fig. 3C) or a fragment thereof. Accordingly, suitable peptides may have the sequence Tyr-Xaa1-Tyr-Xaa2-Ala-Pro-Xaa3-Xaa4-Phe-Xaa5-Xaa6-Phe or a portion thereof, wherein Xaa1-6 may be any amino acid radical. Xaa1 preferably is a serine radical or a similar amino acid. Xaa2 preferably is an aspartate radical or a similar amino acid. Xaa3 preferably is a serine radical or a similar amino acid. Xaa4 preferably is an aspartate radical or a similar amino acid. Xaa5 preferably is an isoleucine radical or a similar amino acid. Xaa6 preferably is an asparagine radical or a similar amino acid. A particularly preferred portion is the sequence Tyr-Xaa1-Tyr-Xaa2-Ala-Pro-Xaa3-Xaa4-Phe. By similar amino acid is meant an amino acid that is considered to result in a conservative change of the peptide's structure when it replaces the amino acid to which it is similar. For instance, aspartate is similar to glutamate. The peptide preferably has a length of 3 to 15, more preferably of 4 to 10 and advantageously of 5 to 8 amino acid, the sum of $n + m$ thus being 2 to 14, more preferably of 3 to 9 and advantageously of 4 to 7, respectively.

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R^3 preferably is a radical different from hydrogen and advantageously represents alkylene- R^9 , alkenylene- R^9 , or alkynylene- R^9 . In this context, the main chain connecting the indene or indole moiety with residue R^9 preferably is relatively long. Accordingly, it is preferred that the main chain of the alkylene radical, alkenylene radical or alkynylene radical contains 3 to 8, e.g. 4, carbon atoms. Said alkylene radical, alkenylene radical and alkynylene radical may be branched. Linear radicals are preferred. Specific examples of said radicals include prop-1,3-ylene, but-1,4-ylene, pent-1,5-ylene and hex-1,6-ylene, with but-1,4-ylene being preferred.

25 R^9 preferably represents aryl or heteroaryl. Specific examples of aryl and heteroaryl radicals include phenyl, naphthyl, indenyl, pyridyl, and indolyl, with pyridyl, e.g. pyrid-2-yl, being preferred.

A specific example of such a preferred residue R^3 is a radical of the formula (IV)



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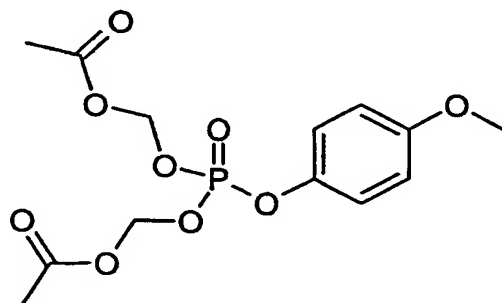
While residues R^4 , R^5 , R^6 and R^7 all may be hydrogen, it is preferred that at least one of said residues, especially R^6 , is different from hydrogen.

R^5 and/or R^6 preferably represent OR^{10} , NHR^{10} , SR^{10} , or alkylene- R^{10} . In this context, the preferred embodiments regarding the alkylene radical are those as described in connection with residues R^1 and R^2 .

R^{10} preferably represents aryl or substituted aryl. In this context, aryl is preferably phenyl. Substituted aryl, in general, contains 1, 2 or 3 substituents which may be the same or different, mono-substitution being preferred. The substituents are preferably selected from the group consisting of hydroxy, $-OPO_3H_2$, $-CH_2PO_3H_2$, $-CF_2PO_3H_2$, $-COOH$, $-CH(COOH)_2$, $-OPO_3(R^{11})_2$, $-CH_2OPO_3(R^{11})_2$, $-CF_2PO_3(R^{11})_2$, $-COOR^{11}$, and $-CH(COOR^{11})_2$, wherein R^{11} is a radical that is cleavable *in vivo*, converting the carboxylic acid esters, phosphate and phosphonate esters to carboxylates, phosphates or phosphonates, respectively. Suitable examples of R^{11} residues are alkyl, CH_2OCO -alkyl, and C_2H_4-S-CO -alkyl. Especially preferred substituents are selected from the group consisting of $-OPO_3H_2$, $-CH_2PO_3H_2$, $-CF_2PO_3H_2$, $-OPO_3(R^{11})_2$, $-CH_2OPO_3(R^{11})_2$, and $-CF_2PO_3(R^{11})_2$. A preferred example of a R^{11} residue is $-CH_2OCO$ -alkyl, alkyl being linear or branched and having 1 to 6 carbon atoms, e.g. methyl.

20

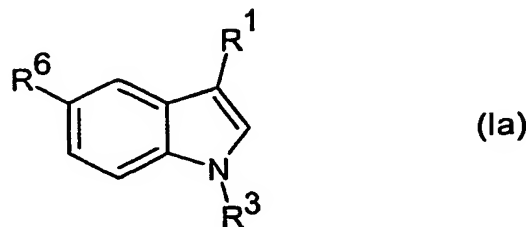
A specific example of such preferred residues R^5 and/or R^6 is the radical of formula (V)



(V)

According to a specific embodiment, the present invention relates to indole derivatives of formula (Ia)

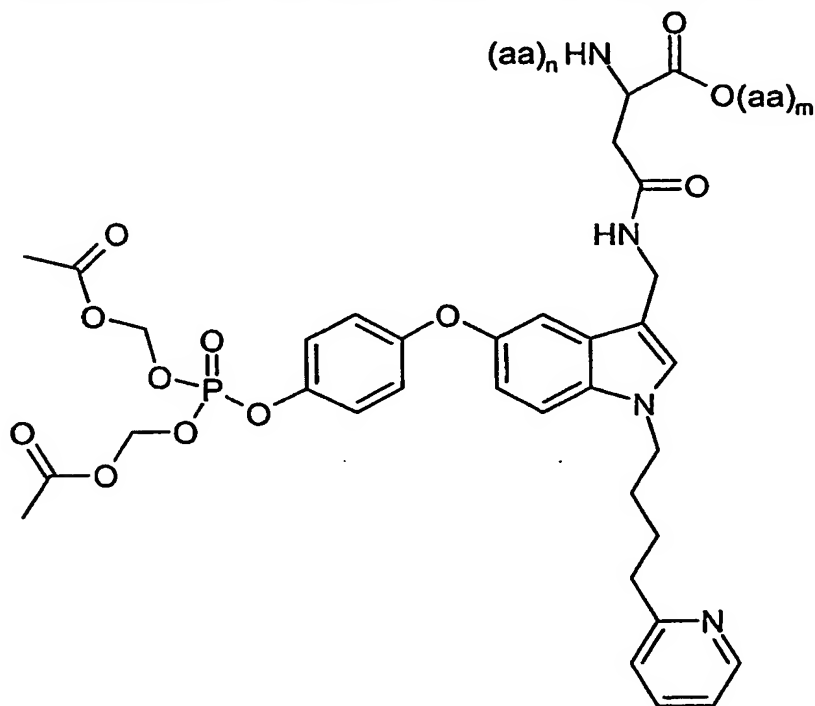
25



wherein

- 5 R^1 , R^3 and R^6 are defined as above,
and optical isomers, physiologically acceptable salts and prodrugs thereof.

A preferred indole derivative of the present invention has the formula (1)



10

wherein

aa , n and m are defined as above.

- 15 The indene and indole derivatives of formula (I) can be prepared by methods well-known to those skilled in the art.

The present invention is further directed to a method for treating cancer, in particular breast and colon carcinomas, comprising administering an effective amount of an Aurora-A

modulator, such as the indole and indene derivatives as described herein, preferably an antagonist or partial antagonist, identified by a computational process of the invention.

5 The compounds according to the invention are thus suitable for the treatment of disorders in which the interaction of Aurora-A with TPX2 is responsible for the formation or the progressive course of these disorders. In particular, the compounds according to the invention can be used for the treatment of cancer.

10 The compounds according to the invention can either be administered as individual therapeutic active compounds or as mixtures with other therapeutic active compounds: they can be administered as such, but in general they are administered in the form of pharmaceutical compositions, i.e. as mixtures of the active compounds with pharmaceutically acceptable excipients, in particular vehicles or diluents and/or additives. The compounds or compositions can be administered enterally, e.g. orally or rectally, or 15 parenterally, e.g. subcutaneously, intravenously or intramuscularly.

The nature of the pharmaceutical composition and of the pharmaceutical carrier or diluent depends on the desired manner of administration. Oral compositions can be present, for example, as tablets or capsules and can contain customary excipients, such as binding 20 agents (e.g. syrup, acacia, gelatin, sorbitol, tragacanth or polyvinylpyrrolidone), fillers (e.g. lactose, sugar, maize starch, calcium phosphate, sorbitol or glycine), lubricants (e.g. magnesium stearate, talc, polyethylene glycol or silica), disintegrating agents (e.g. starch) or wetting agents (e.g. sodium laurylsulphate). Oral liquid preparations can be present in the form of aqueous or oily suspensions, solutions, emulsions, syrups, elixirs or sprays etc. or 25 can be present as dry powders for reconstitution with water or another suitable carrier. Liquid preparations of this type can contain customary additives, for example suspending agents, flavourings, diluents or emulsifiers. For parenteral administration, solutions or suspensions with customary pharmaceutical carriers can be employed.

30 The following examples are to illustrate the invention, but should not be interpreted as a limitation thereon.

Examples

Experimental Procedures

Protein and Antibody Preparation

- Aurora Δ N was cloned in pET M11 (residues 122-403, wild-type and D274N) were expressed in CodonPlus RIL *E.coli* (Stratagene) and purified with TALON resin (Clontech) using manufacturer's instructions. Aurora Δ N was treated with TEV protease to remove the His tag, passed through a TALON column to remove TEV and then purified to homogeneity by size exclusion chromatography. Human and *Xenopus* GST TPX2 fragments were expressed in BL21(DE3) *E.coli*. TPX2 proteins were purified using glutathione sepharose (Pharmacia).
- To form the Aurora Δ N-TPX2 complex, cell lysate from *E.coli* expressing GST TPX2 was passed through a glutathione sepharose column, washed, and then purified Aurora Δ N was passed through the same column. Column resin was incubated with TEV protease to elute the complex, which was further purified by size exclusion chromatography.
- The polyclonal antibody against full-length TPX2 was produced in rabbits with bacterially expressed GST TPX2 (Wittmann et al., 2000) and affinity purified. The 1C1 monoclonal anti-*Xenopus* Aurora-A is described in: Giet R, Uzbekov R, Cubizolles F, Le Guellec K, Prigent C., J Biol Chem. (1999) 274, 15005-13. The polyclonal anti-human Aurora-A was obtained by injecting rabbits with bacterially expressed full-length human Aurora-A.

20

HeLa cell extract and *Xenopus* egg extract preparation

- HeLa cells (CCL2; ATCC, Manassas, VA) were grown in 10% fetal calf serum (FCS) and 2 mM L-glutamine in modified Eagle's medium at 37°C and 5% CO₂. Cells were arrested in S phase using a double thymidine (2 mM) block as described (Stein, 1994) and released from S phase by washing away the thymidine. After 10 h, cells were trypsinized, incubated for 10 min in ice-cold lysis buffer (25 mM Tris pH 7.6, 200 mM NaCl, 1% Triton, protease inhibitors), and centrifuged for 10 min at 15,000 g. *Xenopus* cytosolic factor arrested extracts (CSF extracts) were prepared as described (Murray, 1991).

30 *In vitro* kinase assay

- Full-length TPX2, TPX2(1-43) or TPX2(15-43) at 4 μ M were incubated with full length Aurora-A or Aurora Δ N in kinase buffer (20 mM Hepes pH 7.5, 200 mM KCl, 5 mM MgCl₂, 0.5 mM EGTA, 1 mM DTT, 0.05 % Triton X-100, 50 μ M ATP) containing γ ³²P-ATP (Amersham) in the presence or absence of histone H3 (0.2 mg/ml, Roche), for 15 min at 25°C. For cleavage, GST TPX2(1-43) was incubated with TEV 16-18h at 4° C (Figure 2C) or by adding TEV after the kinase reaction and incubating 10 min at 30° C (Figure 1D). In Figure 2D, Aurora Δ N (8 μ M) was incubated in kinase buffer containing histone H3 and γ ³²P-

ATP for 15 min at 25° C. After separation by SDS-PAGE, phosphorylated histone H3 and TPX2 proteins were detected by autoradiography.

Phosphatase assay

- 5 Active human Aurora-A (2 μ M) was incubated with TPX2, TPX2(1-43) or TPX2(15-43) (3 μ M) for 10 min at 4°C. Samples were diluted in phosphatase buffer (50 mM Tris-HCl pH 7, 0.1 mM EDTA, 1 mM MnCl₂, 5 mM caffeine, 5 mM DTT, 0.025% Tween 20) and incubated in the absence or presence of PP1 (α isoform, NEB) for 0.5h at 30°C. Afterwards proteins were separated by SDS-PAGE and analyzed by Western blotting with anti-Aurora-A or anti-phospho-Aurora-A (Cell Signalling, 1:10000 dilution).

Immunoprecipitation

- For coating beads with anti-GST, 6 μ g of antibody were incubated with 20 μ l of protein A-conjugated Dynabeads 280 (Dyna) in a total volume of 100 μ l PBS-T (PBS, 0.1 % Triton X-100), for at least 1 h at 4°C. The beads were washed twice with PBS-T and twice with HeLa cells lysis buffer or CSF-XB (10 mM Hepes pH 7.7, 50 mM sucrose, 100 mM KCl, 2 mM MgCl₂, 0.1 mM CaCl₂ and 5 mM EGTA). 50 μ l extract was incubated with GST, GST TPX2 1-43, GST TPX2 15-43, GST TPX2 *Xenopus* or GST TPX2(1-39) *Xenopus* proteins (final concentrations: 250 nM *Xenopus*; 1 μ M HeLa) in the absence or presence of RanQ69L-GTP (16 μ M) for 15 minutes at 20 °C and then added to the beads. After 1 h incubation on ice, the beads were washed twice with lysis buffer or CSF-XB, washed twice with PBS-T and boiled in SDS-PAGE sample buffer. The samples were then subjected to gel electrophoresis and analyzed by Western blotting with anti-GST, anti-*Xenopus* TPX2, anti-*Xenopus* Aurora-A or anti-human Aurora-A.

In vitro pull-down assays

- GST or GST TPX2(1-43) (240 μ g) was bound to 100 μ l glutathione sepharose (Pharmacia) in 1ml binding buffer (PBS, 0.05% Tween-20, 2 mM DTT) for 0.5 h. Beads were washed three times, divided into four equal quantities in 1 ml binding buffer and 35 μ g full-length human Aurora-A, Aurora Δ N or Aurora Δ N(D274N) was added. After binding for 0.5 h at 4°C, the resin was washed four times, then incubated overnight in 50 μ l binding buffer plus 2 μ g TEV protease. 10 μ l supernatant from each was analysed by SDS-PAGE. TEV cleavage was necessary because Aurora Δ N and GST TPX 1-43 co-migrate by SDS-PAGE.

Crystallographic methods

Needle-like crystals of AuroraΔN in complex with TPX2 1-43, approximately 10 μm in thickness, were grown at 18°C by vapour diffusion using 18% (w/v) PEG8000, 100 mM MES pH 6.5, 200 mM MgSO₄ as well buffer and hanging drops comprising a 1:1 mix of 20 mg/ml complex pre-mixed with 2 mM ATP_γS and 0.2 mM MgSO₄, and 20% PEG8000, 100 mM MES pH 6.5, 200 mM MgSO₄. For cryo-protection, the drop buffer was supplemented with 17.5% (v/v) glycerol. Hexagonal prism crystals of the wild-type AuroraΔN kinase alone, approximately 50 μm in all dimensions, were grown by vapour diffusion using 20% PEG300, 5% PEG8000, 100 mM Tris 8.5, 10% glycerol as well buffer and sitting drops comprising a 1:1 mix of well buffer and 9 mg/ml protein pre-incubated with 2 mM ATP_γS and 2 mM MgSO₄. Diffraction data were collected at 100K and processed using the CCP4 suite of programs (CCP4, 1994). Structures were solved by molecular replacement using CNS (Brunger et al., 1998) and the coordinates of the cAMP-dependent protein kinase catalytic subunit as an initial model (Mashhoon et al., 2001). CNS was used for refinement and O (Jones et al., 1991) for model building. The statistics for data collection and refinement are shown in Table 1. Structure figures were prepared using PyMOL (DeLano, 2002). Coordinates and structure factors have been deposited in the Protein Data Bank with accession codes 1ol7 and 1ol5 for phosphorylated AuroraΔN alone and in complex with TPX2(1-43), respectively.

20 Mapping of a minimal domain of TPX2 sufficient for binding and activating Aurora-A
A minimal domain of TPX2 sufficient to interact with Aurora-A was mapped. The Aurora-A binding domain of TPX2 resides within its N-terminal 150 residues. Inspection of a sequence alignment of TPX2 shows that only a third of this region is conserved across species (residues 1-43 in human TPX2, 1-39 in *Xenopus* TPX2). This fragment is able to co-immunoprecipitate Aurora-A from *Xenopus* egg extracts to the same extent as the full-length protein (Figure 1A, lanes 6 and 4 respectively). In the egg extracts, efficient binding of TPX2 to Aurora-A requires Ran locked into its GTP-bound form (RanQ69L), which releases TPX2 from a complex with importin α/β. *Xenopus* TPX2(1-39) binds Aurora-A in a RanGTP-independent manner (Figure 1A, lanes 5 and 6), consistent with it lacking the portion of TPX2 regulated by Ran. The corresponding fragment of human TPX2 (residues 1-43) is able to interact with Aurora-A using pull-down experiments in HeLa extract, while a shorter construct encompassing residues 15-43 is unable to do so (Figure 1B, lanes 2 and 3 respectively).

35 The minimal Aurora-A binding domain of human TPX2(1-43) is sufficient to stimulate the activity of the kinase *in vitro* (Figure 1C). Phosphorylation of histone H3, an Aurora-A substrate, is markedly increased by the addition of TPX2(1-43) (Figure 1C compare lane 1

with lane 3), but not by the shorter TPX2(15-43) (lane 4). Full-length TPX2 also increases the activity of the kinase, but appears less effective than the fragment. Full-length TPX2 may require additional factors such as microtubules for full activation. While microtubules can stimulate TPX2 activation of Aurora-A, no enhancement is detected for TPX2 1-43, which does not bind microtubules. Full-length TPX2 is itself a substrate for Aurora-A. The phosphorylation observed for GST-fused TPX2(1-43) (Figure 1C, lane 3) is however likely a non-specific artifact of the *in vitro* reaction because upon cleavage of the fusion protein phosphorylation signal is also detected on GST (lane 2). Furthermore, mass spectroscopy does not reveal Aurora-A phosphorylation sites in full-length TPX2.

The presence of TPX2(1-43) protects Aurora-A from deactivating dephosphorylation (Figure 1E). In the absence of TPX2, Aurora-A is completely dephosphorylated by phosphatase PP1 (lanes 1 and 2). In the presence of full-length TPX2, PP1 treatment dephosphorylates most sites of Aurora-A (lanes 3 and 4, upper panel) but prevents dephosphorylation of Thr288^{AUR} (lane 4, lower panel, arrow). An even stronger protection effect is observed upon addition of TPX2(1-43) (lane 6). In the presence of TPX2 15-43, Aurora-A is fully dephosphorylated as in the absence of TPX2 altogether (lanes 8 and 2), consistent with the shorter fragment being unable to bind Aurora-A (Figure 1B). Thus, residues 1-43 of human TPX2 are necessary and sufficient for Aurora-A binding, activation and protection from dephosphorylation.

Overall structure of TPX2-bound Aurora-A

For crystallisation purposes, a minimal functional complex of Aurora-A and TPX2 was focused on. The N-terminus of Aurora-A is overall poorly conserved across species and is not required to bind TPX2. A fragment of Aurora-A lacking the N-terminus (residues 122-403, Aurora Δ N) interacts with the active fragment of TPX2 (1-43) as efficiently as the full-length kinase (Figure 2A lanes 5 and 4). Both fragments are highly conserved (Figure 2D, 2E) and indeed *Xenopus* TPX2(1-39) can bind human Aurora Δ N. Aurora Δ N is phosphorylated when expressed in *E. coli*, as detected by a phospho-specific antibody (Figure 2B, lane 1). This appears to be due to Aurora-A autophosphorylation rather than to the activity of a bacterial kinase, since no phosphorylation can be detected upon expressing a mutant where an important catalytic residue, Asp274^{AUR}, has been mutated to Asn (Figure 2B, lane 2). The unphosphorylated mutant is catalytically inactive but retains TPX2-binding activity (Figure 2A, lane 6). Aurora Δ N is activated by TPX2(1-43) (Figure 2C, lanes 2,3).

The complex between human phosphorylated Aurora Δ N and TPX2(1-43) is active in histone H3 phosphorylation (Figure 2C, lane 7). The complex was crystallized in the presence of

Mg²⁺ ions and the ATP analogue ATP γ S. The structure was determined by molecular replacement and refined it using 2.5 Å resolution data to a *R*_{free} of 25.2% (see Table 1). The polypeptide model includes the catalytic core of the kinase (residues 123-387^{AUR}) and two segments of TPX2 (residues 7-21^{TPX} and 30-43^{TPX}). No ordered electron density is present for the eight intervening residues of TPX2 (22-29^{TPX}), which have therefore not been modelled.

The kinase catalytic core has an overall bilobate structure (Figure 3A,B). Briefly, the N-terminal lobe (residues 123-210) consists of a β -sheet and two α -helices, including the prominent helix α C whereas the C-terminal and larger lobe (residues 217-387) is mostly α -helical. The active site is situated at the interface between the lobes and includes the ATP-binding site, the catalytic base (Asp256^{AUR}) and the kinase activation segment (residues 274-299^{AUR}). In contrast to the structure of unphosphorylated Aurora-A, the activation segment is well ordered in the electron density and includes two phosphorylated threonine residues (Thr287^{AUR} and Thr288^{AUR}). Although the crystals were formed in the presence of ATP- γ S, the electron density for the nucleotide reveals only the adenosine with two ordered phosphates and has been modelled as an ADP.

Specific recognition of TPX2 at two sites on Aurora-A

TPX2 binds Aurora-A with two separate stretches recognized at two distinct sites on the kinase. The upstream stretch (residues 7-21^{TPX}) binds at the N-terminal lobe of Aurora-A (Figure 3A,B). The downstream stretch (residues 30-43^{TPX}) binds in a α -helical conformation between the N- and C-terminal lobes (Figure 3A,B). The two Aurora-A-binding motifs of TPX2 appear to be connected by a flexible linker (disordered in the structure) that is variable in length and sequence across species (Figure 2D). Additionally, the two stretches are connected by an intramolecular hydrogen bond between Asp11^{TPX} and Trp34^{TPX}.

The upstream stretch of TPX2 has a mostly extended conformation, with a kink in the middle induced at a proline residue (Pro13^{TPX}) (for details see Figure 3C). The conserved segment ⁸YSYDAPS¹⁴ (Figure 2D) is engaged in extensive main-chain and side-chain interactions with Aurora-A. In particular, Tyr8^{TPX}, Tyr10^{TPX} and Ala12^{TPX} tightly nestle into a hydrophobic groove between the β -sheet, helix α B and helix α C. An adjacent hydrophobic groove accommodates the side chains of TPX2 residues from Phe16^{TPX} to Phe19^{TPX}. The N-terminal residues of the Aurora-A catalytic core make key contributions to this interface, in particular with Arg126^{AUR} forming a cation- π interaction with Phe16^{TPX}.

The downstream helical stretch of TPX2 interacts with both helix α C and the activation segment of Aurora-A, bridging them (see Figure 3D for details). Most prominently, two conserved aromatic residues (Trp34^{TPX} and Phe35^{TPX}) interact with His187^{AUR} and His280^{AUR}, and Ala39^{TPX} additionally contacts the activation segment at Pro282^{AUR}. While
 5 the side of the TPX2 helix in contact with the kinase is lined by hydrophobic and conserved residues, the opposite side exposed to solvent comprises hydrophilic and variable residues. Residues 40-43^{TPX} at the end of the helix assume an extended conformation and are involved in contacts with a symmetry-related Aurora-A molecule within the crystal lattice.

10 TPX2 is phosphorylated in mitotic extracts and may well be regulated by phosphorylation. Even if TPX2 was phosphorylated in the first 43 residues, examination of the crystal structure suggests that the interaction of TPX2 with Aurora-A is unlikely to be regulated this way because all the conserved serine residues point towards solvent.

15

Phosphorylated Aurora-A is in an active conformation when bound to TPX2

Comparison with other kinase structures reveals that phosphorylated TPX2-bound Aurora-A closely matches the conformation of kinases in the active conformation. Using the program DALI (Holm and Sander, 1993), it was found particularly similar to cAMP-dependent protein
 20 kinase (PDB code 1YDS, 1.3 Å r.m.s.d., 257 structurally equivalent residues). Structural comparison shows that all the conserved residues at the active site are correctly oriented for catalysis (Figure 4A). These include the positively-charged residue aligning the phosphates for catalysis (Lys162^{AUR}, equivalent to Lys72^{CAPK}), the negatively-charged residue coordinating the magnesium ion bound to the nucleotide (Asp274^{AUR}, equivalent to
 25 Asp184^{CAPK}), and the catalytic base (Asp256^{AUR}, equivalent to Asp166^{CAPK}) whose role is to transfer the γ -phosphate of ATP to the hydroxyl group of a substrate serine or threonine residue.

The phosphorylated activation segment of TPX2-bound Aurora-A is in a conformation typical
 30 of active Ser/Thr kinases. It is virtually superposable to that of active cAPK (Figure 4A), with an r.m.s.d. of 0.8 Å between the C α atoms of residues 274-299^{AUR} and 184-208^{CAPK}. In cAPK, the phosphorylated Thr197^{CAPK} interacts with Arg165^{CAPK} and with a basic surface patch (His87^{CAPK} and Lys189^{CAPK}), influencing the preceding catalytic residue (Asp166^{CAPK}). In Aurora-A, the phosphoryl moiety of Thr288^{AUR} is at the same structural position and interacts
 35 with the corresponding Arg255^{AUR} and with a similar, though not identical, basic patch (Arg180^{AUR} and Arg286^{AUR}), linking the catalytic residue (Asp256^{AUR}) to helix α C and to the activation segment. Mutation of Thr288^{AUR} to Asp generates a protein more active than

unphosphorylated wild-type Aurora-A, but much less active than the phosphorylated wild-type kinase. This mutation is thus a poor mimic of phosphorylation at Thr288^{AUR}, and although a Glu may potentially produce a stronger effect by more closely approximating the position of the phosphate, it would also be inadequate to balance the positive charges of the three surrounding arginines.

The phosphorylated activation segment of Aurora-A is in an inactive conformation in the absence of TPX2

To address the contribution of TPX2 to the conformation at the active site of TPX2-bound Aurora-A, the structure of phosphorylated Aurora Δ N has been determined in the absence of TPX2. The model includes residues 127-389^{AUR} and has been refined at 2.75 Å resolution to an *R*_{free} of 29.6% (Table 1). The overall structure of phosphorylated Aurora-A is similar for the TPX2-bound and unbound forms. The two lobes of the kinase have the same relative orientation and helix α C does not change conformation upon binding the regulator (Figure 4A). Overall, more than 95% of the amino-acid residues superpose with an overall r.m.s.d. of 0.9 Å. However, the two structures differ significantly in the activation segment.

The phosphorylated activation segments of Aurora-A in the TPX2-bound state (Figure 4A) and unbound state (Figure 4A) diverge between residues His280^{AUR} and Leu293^{AUR} (rmsd of 5.4 Å). In the absence of TPX2, the phosphorylated Thr288^{AUR} is exposed to solvent rather than pointing towards Arg255^{AUR} as observed when TPX2 is bound (Figure 4A). The region of the activation segment around the phosphorylated Thr288^{AUR} (residues 286-291^{AUR}) is relatively disordered, with average B-factors of 85 Å² as compared with 53 Å² for the rest of the molecule. However, the tracing of the polypeptide chain is unambiguous and this fragment of the activation segment is overall less closely packed to the C-terminal lobe of the kinase. The segment becomes well ordered again at Thr292^{AUR} and Leu293^{AUR}. This part of the activation segment is in a different conformation with respect to the TPX2-bound form (Figure 4A), with Thr292^{AUR} being unable to hydrogen bond and thus influence the catalytic Asp256^{AUR} (Figure 4A). This conformation seems to be stabilized by the movement of Leu293^{AUR}, which inserts its side chain into a small apolar pocket. The presence of a Leu at this position is uncommon in other kinases, which typically have a Pro residue instead (cAPK, for example, Figures 2E). A further movement of residues 298-306 accommodates changes in the adjacent activation segment, and leads to the formation of a Glu302-His366 interaction. This interaction may be affected by the negative charge introduced in the S349D mutant of *Xenopus* Aurora-A explaining why this mutant is catalytically inactive.

Structural basis for the activation of Aurora-A by TPX2

Comparison of phosphorylated Aurora-A in the unbound and TPX2-bound forms reveals the molecular basis for the enhancement of kinase activity. In the absence of TPX2, the crucial phosphothreonine does not bind to helix α C and the activation segment overlaps with the substrate-binding site rather than providing a substrate-binding platform. The phosphorylated Thr288^{AUR} has no direct connection with TPX2, the phosphate moiety being 14 Å from the nearest TPX2 atom. Nonetheless, TPX2 induces a 10 Å movement of the phosphoryl moiety required to achieve the active conformation (Figure 4B).

The helical stretch of TPX2 contacts the activation segment at His280^{AUR} and Pro282^{AUR}, which appear to be the pivot points of the conformational change (Figures 4B, 4C). In essence, a rotation about His280^{AUR} swings Pro282^{AUR} and Ser283^{AUR} towards the TPX2 helix, pulling downstream residues of the activation segment to pack more closely with the kinase core (Figure 4B). In this lever-arm-like mechanism, a small change at the pivot points (His280^{AUR}, Pro282^{AUR}) produces a large movement in the arm (P-Thr288^{AUR} Figure 4C). While in the unbound form the activation segment is rather mobile and has probably sufficient conformational freedom to adopt an active conformation in the presence of substrate (basal kinase activity, Figure 1C, lane 1), in the TPX2-bound form, the active conformation is ready for substrate binding and catalysis (increased kinase activity, Figure 1C, lanes 2 and 3). The C-terminal residues (40-43^{TPX}) protruding from a neighbouring TPX2 molecule in the crystals bind to the activation segment, albeit in the opposite main chain direction to a real substrate. Substrate binding alone does not fully activate Aurora-A in solution (Figure 1C), and it is therefore very unlikely that this substrate-like contact is responsible for the active conformation in the crystal structure. Substrate binding, however, might assist in inducing an active conformation, especially in the absence of TPX2.

In addition to enhancing the activity of Aurora-A, TPX2 also protects the kinase from dephosphorylation by phosphatases. The site for PP1 binding on Aurora-A is mapped to the C-terminus, a region that is distant from the TPX2 binding site and that is structurally unaffected upon binding of the regulator. Thus TPX2 is unlikely to protect Aurora-A from dephosphorylation by preventing phosphatase binding. Indeed, even in the presence of TPX2, the phosphatase is capable of removing the phosphates from most side chains with the exception of Thr288^{AUR} (Figure 1E). TPX2 prevents Thr288^{AUR} dephosphorylation by moving the phosphate moiety from a solvent-exposed position to a buried position, which is inaccessible to an incoming phosphatase. The other phosphorylated threonine in the kinase catalytic core, Thr287^{AUR}, is conspicuously exposed to solvent and may serve as a decoy to further mask Thr288^{AUR} (Figure 3B).

Table 1. Summary of crystallographic analysis

		Phospho- Aurora-A + TPX2	Phospho- Aurora-A
5	Crystals		
	Spacegroup	<i>P2₁2₁2₁</i>	<i>P6₁22</i>
	Lattice constants		
	<i>a</i> (Å)	59.63	81.18
	<i>b</i> (Å)	81.72	81.18
	<i>c</i> (Å)	83.05	169.62
10	Data collection		
	X-ray source	SLS XO6SA	ESRF ID14EH1
	Resolution range (Å)	40-2.5	70-2.75
	(Highest resolution shell)	(2.64-2.5)	(2.9-2.75)
15	Unique reflections	14609	9235
	Completeness(%)	100 (100)	100 (100)
	Multiplicity	5.6 (5.7)	10.1 (10.6)
	Rmerge (%)	9.9 (24.8)	11.9 (34.6)
	<i>I</i> / σ (<i>I</i>)	5.1 (1.1)	3.8 (2.1)
20	Refinement		
	Resolution range (Å)	40-2.5	20-2.75
	Number of residues	294	263
	Number of waters	144	9
25	<i>R</i> factor (%)	19.4	25.7
	<i>R</i> free ^a (%)	25.2	29.6
	Ramachandran plot		
	Most favoured (%)	91.5	82.4
30	Allowed (%)	8.1	16.3
	Generously allowed (%)	0.0	0.9
	Forbidden (%)	0.4 ^b	0.4 ^b

35 ^a Free *R*factor was computed using 5% of the data assigned randomly (Brunger, 1992).

^b Ser226^{AUR} resides in a loop and the conformation is supported by excellent electron density.

ATOM C	1	CB	GLN A 127	267.519	-61.189	87.734	1.00	66.58	A
ATOM C	2	CG	GLN A 127	266.971	-61.391	86.330	1.00	76.29	A
ATOM C	3	CD	GLN A 127	266.372	-60.121	85.741	1.00	79.34	A
ATOM O	4	OE1	GLN A 127	265.589	-60.183	84.781	1.00	82.34	A
ATOM N	5	NE2	GLN A 127	266.735	-58.962	86.307	1.00	82.40	A
ATOM C	6	C	GLN A 127	269.192	-59.883	89.051	1.00	63.35	A
ATOM O	7	O	GLN A 127	269.877	-58.853	89.024	1.00	70.04	A
ATOM N	8	N	GLN A 127	269.910	-61.949	87.808	1.00	58.04	A
ATOM C	9	CA	GLN A 127	269.002	-60.755	87.810	1.00	67.74	A
ATOM N	10	N	TRP A 128	268.566	-60.307	90.137	1.00	61.21	A
ATOM C	11	CA	TRP A 128	268.621	-59.552	91.366	1.00	53.96	A
ATOM C	12	CB	TRP A 128	267.315	-59.733	92.133	1.00	50.38	A
ATOM C	13	CG	TRP A 128	266.140	-59.256	91.369	1.00	49.11	A
ATOM C	14	CD2	TRP A 128	265.908	-57.928	90.897	1.00	50.34	A
ATOM C	15	CE2	TRP A 128	264.697	-57.962	90.150	1.00	53.33	A
ATOM C	16	CE3	TRP A 128	266.611	-56.713	91.017	1.00	53.44	A
ATOM C	17	CD1	TRP A 128	265.096	-60.014	90.921	1.00	47.17	A
ATOM N	18	NE1	TRP A 128	264.228	-59.249	90.191	1.00	49.20	A
ATOM C	19	CZ2	TRP A 128	264.160	-56.816	89.514	1.00	56.77	A
ATOM C	20	CZ3	TRP A 128	266.094	-55.571	90.392	1.00	60.23	A
ATOM C	21	CH2	TRP A 128	264.869	-55.633	89.639	1.00	61.57	A
ATOM C	22	C	TRP A 128	269.787	-59.909	92.262	1.00	54.43	A
ATOM O	23	O	TRP A 128	270.317	-61.026	92.231	1.00	54.76	A
ATOM N	24	N	ALA A 129	270.184	-58.955	93.085	1.00	55.48	A
ATOM C	25	CA	ALA A 129	271.283	-59.206	94.006	1.00	60.01	A
ATOM C	26	CB	ALA A 129	272.608	-58.800	93.341	1.00	66.60	A
ATOM C	27	C	ALA A 129	271.010	-58.371	95.258	1.00	56.86	A
ATOM O	28	O	ALA A 129	270.365	-57.326	95.173	1.00	59.08	A
ATOM N	29	N	LEU A 130	271.517	-58.821	96.401	1.00	51.68	A
ATOM C	30	CA	LEU A 130	271.314	-58.126	97.665	1.00	53.06	A

5	ATOM C	31	CB	LEU A 130	272.108	-58.770	98.787	1.00	43.18	A
	ATOM C	32	CG	LEU A 130	272.080	-58.110	100.164	1.00	36.68	A
	ATOM C	33	CD1	LEU A 130	270.621	-57.934	100.570	1.00	47.13	A
	ATOM C	34	CD2	LEU A 130	272.839	-58.975	101.186	1.00	38.64	A
10	ATOM C	35	C	LEU A 130	271.750	-56.702	97.591	1.00	55.17	A
	ATOM O	36	O	LEU A 130	271.223	-55.834	98.305	1.00	61.19	A
15	ATOM N	37	N	GLU A 131	272.686	-56.469	96.690	1.00	58.94	A
	ATOM C	38	CA	GLU A 131	273.276	-55.172	96.539	1.00	57.04	A
20	ATOM C	39	CB	GLU A 131	274.689	-55.400	96.030	1.00	63.45	A
	ATOM C	40	CG	GLU A 131	275.441	-56.450	96.938	1.00	73.38	A
	ATOM C	41	CD	GLU A 131	275.249	-57.909	96.486	1.00	79.54	A
	ATOM O	42	OE1	GLU A 131	274.529	-58.142	95.477	1.00	80.97	A
25	ATOM O	43	OE2	GLU A 131	275.838	-58.820	97.135	1.00	88.53	A
	ATOM C	44	C	GLU A 131	272.458	-54.235	95.682	1.00	55.07	A
30	ATOM O	45	O	GLU A 131	272.851	-53.119	95.439	1.00	51.83	A
	ATOM N	46	N	ASP A 132	271.280	-54.704	95.299	1.00	53.60	A
35	ATOM C	47	CA	ASP A 132	270.298	-53.994	94.487	1.00	58.59	A
	ATOM C	48	CB	ASP A 132	269.514	-54.987	93.656	1.00	69.09	A
	ATOM C	49	CG	ASP A 132	270.030	-55.141	92.284	1.00	68.36	A
	ATOM O	50	OD1	ASP A 132	269.776	-54.250	91.447	1.00	73.44	A
40	ATOM O	51	OD2	ASP A 132	270.704	-56.159	92.048	1.00	76.16	A
	ATOM C	52	C	ASP A 132	269.267	-53.412	95.449	1.00	59.74	A
45	ATOM O	53	O	ASP A 132	268.472	-52.547	95.093	1.00	56.43	A
	ATOM N	54	N	PHE A 133	269.239	-53.925	96.666	1.00	62.15	A
50	ATOM C	55	CA	PHE A 133	268.239	-53.448	97.598	1.00	62.91	A
	ATOM C	56	CB	PHE A 133	267.324	-54.622	97.974	1.00	59.55	A
55	ATOM C	57	CG	PHE A 133	266.737	-55.337	96.775	1.00	61.26	A
	ATOM C	58	CD1	PHE A 133	267.467	-56.312	96.095	1.00	60.00	A
60	ATOM C	59	CD2	PHE A 133	265.442	-55.059	96.346	1.00	60.03	A
	ATOM C	60	CE1	PHE A 133	266.910	-56.996	94.991	1.00	65.06	A
	ATOM C	61	CE2	PHE A 133	264.883	-55.719	95.264	1.00	60.82	A

5	ATOM C	62	CZ	PHE	A	133	265.607	-56.697	94.585	1.00	61.32	A
	ATOM C	63	C	PHE	A	133	268.740	-52.733	98.847	1.00	61.07	A
10	ATOM O	64	O	PHE	A	133	269.866	-52.972	99.318	1.00	66.24	A
	ATOM N	65	N	GLU	A	134	267.878	-51.829	99.340	1.00	59.55	A
15	ATOM C	66	CA	GLU	A	134	268.062	-51.035	100.573	1.00	58.90	A
	ATOM C	67	CB	GLU	A	134	267.589	-49.593	100.353	1.00	54.77	A
20	ATOM C	68	CG	GLU	A	134	268.478	-48.772	99.488	1.00	63.45	A
	ATOM C	69	CD	GLU	A	134	268.205	-47.282	99.556	1.00	61.84	A
25	ATOM O	70	OE1	GLU	A	134	268.808	-46.576	100.384	1.00	75.06	A
	ATOM O	71	OE2	GLU	A	134	267.388	-46.803	98.768	1.00	73.27	A
30	ATOM C	72	C	GLU	A	134	267.139	-51.698	101.627	1.00	53.85	A
	ATOM O	73	O	GLU	A	134	265.909	-51.607	101.526	1.00	60.03	A
35	ATOM N	74	N	ILE	A	135	267.713	-52.362	102.621	1.00	52.32	A
	ATOM C	75	CA	ILE	A	135	266.917	-53.042	103.625	1.00	50.89	A
40	ATOM C	76	CB	ILE	A	135	267.750	-54.131	104.343	1.00	48.23	A
	ATOM C	77	CG2	ILE	A	135	266.828	-55.078	105.127	1.00	51.35	A
45	ATOM C	78	CG1	ILE	A	135	268.552	-54.940	103.317	1.00	48.00	A
	ATOM C	79	CD1	ILE	A	135	267.731	-55.720	102.398	1.00	35.46	A
50	ATOM C	80	C	ILE	A	135	266.298	-52.129	104.674	1.00	50.54	A
	ATOM O	81	O	ILE	A	135	266.973	-51.281	105.250	1.00	50.32	A
55	ATOM N	82	N	GLY	A	136	265.004	-52.334	104.924	1.00	49.85	A
	ATOM C	83	CA	GLY	A	136	264.286	-51.534	105.903	1.00	44.78	A
60	ATOM C	84	C	GLY	A	136	264.165	-52.255	107.228	1.00	44.85	A
	ATOM O	85	O	GLY	A	136	265.040	-53.071	107.574	1.00	45.10	A
65	ATOM N	86	N	ARG	A	137	263.071	-51.996	107.940	1.00	40.54	A
	ATOM C	87	CA	ARG	A	137	262.891	-52.598	109.248	1.00	47.22	A
70	ATOM C	88	CB	ARG	A	137	261.911	-51.766	110.065	1.00	46.15	A
	ATOM C	89	CG	ARG	A	137	260.481	-51.887	109.585	1.00	46.77	A
75	ATOM C	90	CD	ARG	A	137	259.521	-51.284	110.589	1.00	47.76	A
	ATOM N	91	NE	ARG	A	137	258.174	-51.283	110.058	1.00	44.18	A
80	ATOM C	92	CZ	ARG	A	137	257.364	-52.330	110.097	1.00	49.13	A

5	ATOM N	93	NH1	ARG	A	137	257.779	-53.468	110.655	1.00	50.41	A
	ATOM N	94	NH2	ARG	A	137	256.144	-52.230	109.579	1.00	42.98	A
	ATOM C	95	C	ARG	A	137	262.358	-54.014	109.150	1.00	48.40	A
	ATOM O	96	O	ARG	A	137	261.734	-54.370	108.150	1.00	52.53	A
10	ATOM N	97	N	PRO	A	138	262.589	-54.840	110.190	1.00	48.54	A
	ATOM C	98	CD	PRO	A	138	263.443	-54.581	111.363	1.00	46.06	A
15	ATOM C	99	CA	PRO	A	138	262.108	-56.226	110.213	1.00	46.02	A
	ATOM C	100	CB	PRO	A	138	262.685	-56.765	111.524	1.00	49.55	A
	ATOM C	101	CG	PRO	A	138	263.905	-55.955	111.710	1.00	42.97	A
20	ATOM C	102	C	PRO	A	138	260.561	-56.262	110.207	1.00	49.85	A
	ATOM O	103	O	PRO	A	138	259.920	-55.810	111.142	1.00	50.42	A
25	ATOM N	104	N	LEU	A	139	259.980	-56.799	109.138	1.00	45.75	A
	ATOM C	105	CA	LEU	A	139	258.545	-56.896	109.005	1.00	39.58	A
	ATOM C	106	CB	LEU	A	139	258.181	-57.130	107.558	1.00	37.24	A
30	ATOM C	107	CG	LEU	A	139	258.109	-55.885	106.664	1.00	42.68	A
	ATOM C	108	CD1	LEU	A	139	257.816	-56.315	105.170	1.00	32.13	A
35	ATOM C	109	CD2	LEU	A	139	256.990	-54.961	107.170	1.00	43.77	A
	ATOM C	110	C	LEU	A	139	257.968	-58.002	109.880	1.00	40.81	A
	ATOM O	111	O	LEU	A	139	256.907	-57.861	110.480	1.00	45.92	A
40	ATOM N	112	N	GLY	A	140	258.675	-59.111	109.970	1.00	45.15	A
	ATOM C	113	CA	GLY	A	140	258.198	-60.218	110.789	1.00	48.82	A
45	ATOM C	114	C	GLY	A	140	259.222	-61.317	111.040	1.00	48.37	A
	ATOM O	115	O	GLY	A	140	260.326	-61.310	110.492	1.00	53.08	A
50	ATOM N	116	N	LYS	A	141	258.842	-62.283	111.856	1.00	52.66	A
	ATOM C	117	CA	LYS	A	141	259.740	-63.376	112.192	1.00	56.79	A
	ATOM C	118	CB	LYS	A	141	259.961	-63.404	113.707	1.00	61.89	A
55	ATOM C	119	CG	LYS	A	141	260.862	-64.513	114.210	1.00	68.25	A
	ATOM C	120	CD	LYS	A	141	260.894	-64.538	115.750	1.00	78.79	A
60	ATOM C	121	CE	LYS	A	141	261.863	-65.624	116.242	1.00	83.42	A
	ATOM N	122	NZ	LYS	A	141	261.987	-65.651	117.745	1.00	90.84	A
	ATOM C	123	C	LYS	A	141	259.219	-64.728	111.704	1.00	57.82	A

Atom	Res	Atom	Res	B	B	B	B	B	B	B	B
5	ATOM O	124	O	LYS A 141	258.150	-65.199	112.084	1.00	57.17	A	
	ATOM N	125	N	GLY A 142	259.990	-65.342	110.823	1.00	63.79	A	
	ATOM C	126	CA	GLY A 142	259.627	-66.648	110.315	1.00	67.77	A	
	ATOM C	127	C	GLY A 142	260.381	-67.717	111.087	1.00	68.12	A	
10	ATOM O	128	O	GLY A 142	260.756	-67.533	112.255	1.00	76.19	A	
	ATOM N	129	N	LYS A 143	260.638	-68.829	110.410	1.00	66.29	A	
	ATOM C	130	CA	LYS A 143	261.359	-69.941	111.016	1.00	62.91	A	
15	ATOM C	131	CB	LYS A 143	260.576	-71.221	110.783	1.00	56.50	A	
	ATOM C	132	CG	LYS A 143	260.990	-72.331	111.694	1.00	59.59	A	
20	ATOM C	133	CD	LYS A 143	259.804	-73.170	112.130	1.00	65.95	A	
	ATOM C	134	CE	LYS A 143	260.182	-74.141	113.303	1.00	69.37	A	
	ATOM N	135	NZ	LYS A 143	259.069	-75.109	113.596	1.00	70.95	A	
25	ATOM C	136	C	LYS A 143	262.773	-70.081	110.500	1.00	62.52	A	
	ATOM O	137	O	LYS A 143	263.725	-70.302	111.243	1.00	61.60	A	
30	ATOM N	138	N	PHE A 144	262.909	-69.898	109.200	1.00	68.60	A	
	ATOM C	139	CA	PHE A 144	264.215	-70.021	108.556	1.00	74.62	A	
	ATOM C	140	CB	PHE A 144	264.109	-70.886	107.296	1.00	69.32	A	
35	ATOM C	141	CG	PHE A 144	263.583	-72.278	107.565	1.00	69.58	A	
	ATOM C	142	CD1	PHE A 144	262.211	-72.526	107.690	1.00	66.23	A	
40	ATOM C	143	CD2	PHE A 144	264.460	-73.335	107.731	1.00	63.51	A	
	ATOM C	144	CE1	PHE A 144	261.738	-73.816	107.978	1.00	73.24	A	
	ATOM C	145	CE2	PHE A 144	263.985	-74.608	108.014	1.00	69.83	A	
45	ATOM C	146	CZ	PHE A 144	262.629	-74.850	108.138	1.00	66.31	A	
	ATOM C	147	C	PHE A 144	264.768	-68.665	108.234	1.00	74.80	A	
50	ATOM O	148	O	PHE A 144	265.636	-68.496	107.395	1.00	82.71	A	
	ATOM N	149	N	GLY A 145	264.248	-67.691	108.955	1.00	83.57	A	
	ATOM C	150	CA	GLY A 145	264.676	-66.320	108.782	1.00	77.10	A	
55	ATOM C	151	C	GLY A 145	263.544	-65.296	108.827	1.00	75.14	A	
	ATOM O	152	O	GLY A 145	262.338	-65.557	108.521	1.00	74.64	A	
60	ATOM N	153	N	ASN A 146	263.966	-64.097	109.195	1.00	67.46	A	
	ATOM C	154	CA	ASN A 146	263.050	-62.976	109.318	1.00	65.84	A	

5	ATOM C	155	CB	ASN A 146	263.674	-61.895	110.208	1.00	68.52	A
	ATOM C	156	CG	ASN A 146	263.873	-62.369	111.664	1.00	74.23	A
	ATOM O	157	OD1	ASN A 146	264.045	-63.577	111.946	1.00	76.10	A
	ATOM N	158	ND2	ASN A 146	263.871	-61.415	112.588	1.00	74.93	A
10	ATOM C	159	C	ASN A 146	262.727	-62.402	107.955	1.00	60.10	A
	ATOM O	160	O	ASN A 146	263.442	-62.661	106.979	1.00	60.40	A
15	ATOM N	161	N	VAL A 147	261.651	-61.614	107.909	1.00	49.34	A
	ATOM C	162	CA	VAL A 147	261.208	-60.938	106.697	1.00	34.29	A
	ATOM C	163	CB	VAL A 147	259.691	-61.195	106.433	1.00	35.55	A
20	ATOM C	164	CG1	VAL A 147	259.202	-60.303	105.293	1.00	22.76	A
	ATOM C	165	CG2	VAL A 147	259.444	-62.657	106.040	1.00	25.36	A
25	ATOM C	166	C	VAL A 147	261.432	-59.427	106.905	1.00	36.01	A
	ATOM O	167	O	VAL A 147	261.071	-58.888	107.912	1.00	33.80	A
	ATOM N	168	N	TYR A 148	262.006	-58.743	105.931	1.00	38.73	A
30	ATOM C	169	CA	TYR A 148	262.298	-57.313	106.040	1.00	38.16	A
	ATOM C	170	CB	TYR A 148	263.815	-57.053	105.947	1.00	44.86	A
35	ATOM C	171	CG	TYR A 148	264.625	-57.783	106.981	1.00	51.34	A
	ATOM C	172	CD1	TYR A 148	264.946	-59.110	106.823	1.00	49.12	A
	ATOM C	173	CE1	TYR A 148	265.660	-59.799	107.804	1.00	57.49	A
40	ATOM C	174	CD2	TYR A 148	265.035	-57.152	108.146	1.00	56.42	A
	ATOM C	175	CE2	TYR A 148	265.743	-57.839	109.136	1.00	62.05	A
45	ATOM C	176	CZ	TYR A 148	266.051	-59.159	108.958	1.00	59.22	A
	ATOM O	177	OH	TYR A 148	266.740	-59.818	109.951	1.00	62.90	A
50	ATOM C	178	C	TYR A 148	261.647	-56.485	104.972	1.00	40.31	A
	ATOM O	179	O	TYR A 148	261.240	-56.989	103.910	1.00	39.68	A
	ATOM N	180	N	LEU A 149	261.564	-55.187	105.254	1.00	37.70	A
55	ATOM C	181	CA	LEU A 149	260.992	-54.236	104.287	1.00	36.17	A
	ATOM C	182	CB	LEU A 149	260.495	-52.976	105.019	1.00	38.73	A
60	ATOM C	183	CG	LEU A 149	259.781	-51.920	104.186	1.00	39.39	A
	ATOM C	184	CD1	LEU A 149	258.437	-52.465	103.793	1.00	46.05	A
	ATOM C	185	CD2	LEU A 149	259.655	-50.660	104.957	1.00	40.68	A

	ATOM C	186	C	LEU A 149	262.212	-53.920	103.405	1.00	35.83	A
	ATOM O	187	O	LEU A 149	263.340	-54.217	103.822	1.00	37.60	A
5	ATOM N	188	N	ALA A 150	262.029	-53.321	102.228	1.00	37.02	A
	ATOM C	189	CA	ALA A 150	263.171	-53.041	101.363	1.00	35.35	A
10	ATOM C	190	CB	ALA A 150	263.889	-54.345	100.965	1.00	48.80	A
	ATOM C	191	C	ALA A 150	262.746	-52.334	100.123	1.00	44.17	A
	ATOM O	192	O	ALA A 150	261.665	-52.604	99.566	1.00	41.00	A
15	ATOM N	193	N	ARG A 151	263.619	-51.441	99.666	1.00	47.00	A
	ATOM C	194	CA	ARG A 151	263.319	-50.674	98.468	1.00	50.37	A
20	ATOM C	195	CB	ARG A 151	263.377	-49.171	98.793	1.00	53.91	A
	ATOM C	196	CG	ARG A 151	262.912	-48.272	97.649	1.00	53.96	A
	ATOM C	197	CD	ARG A 151	262.884	-46.817	98.014	1.00	57.39	A
25	ATOM N	198	NE	ARG A 151	264.145	-46.372	98.607	1.00	58.37	A
	ATOM C	199	CZ	ARG A 151	264.561	-45.110	98.572	1.00	58.07	A
30	ATOM N	200	NH1	ARG A 151	263.814	-44.175	97.969	1.00	56.20	A
	ATOM N	201	NH2	ARG A 151	265.718	-44.793	99.131	1.00	55.48	A
	ATOM C	202	C	ARG A 151	264.311	-51.021	97.348	1.00	55.38	A
35	ATOM O	203	O	ARG A 151	265.503	-51.247	97.625	1.00	60.78	A
	ATOM N	204	N	GLU A 152	263.826	-51.059	96.105	1.00	54.28	A
40	ATOM C	205	CA	GLU A 152	264.664	-51.366	94.972	1.00	54.46	A
	ATOM C	206	CB	GLU A 152	263.811	-51.817	93.823	1.00	60.23	A
	ATOM C	207	CG	GLU A 152	264.520	-52.780	92.888	1.00	67.69	A
45	ATOM C	208	CD	GLU A 152	265.617	-52.120	92.087	1.00	75.21	A
	ATOM O	209	OE1	GLU A 152	266.773	-52.020	92.593	1.00	78.70	A
50	ATOM O	210	OE2	GLU A 152	265.305	-51.689	90.951	1.00	76.28	A
	ATOM C	211	C	GLU A 152	265.436	-50.117	94.598	1.00	54.18	A
	ATOM O	212	O	GLU A 152	264.868	-49.045	94.388	1.00	55.50	A
55	ATOM N	213	N	LYS A 153	266.746	-50.275	94.489	1.00	55.96	A
	ATOM C	214	CA	LYS A 153	267.583	-49.115	94.231	1.00	57.21	A
60	ATOM C	215	CB	LYS A 153	269.059	-49.471	94.257	1.00	56.21	A
	ATOM C	216	CG	LYS A 153	269.661	-49.042	95.586	1.00	49.03	A

5	ATOM C	217	CD	LYS A 153	270.821	-49.929	95.975	1.00	56.59	A
	ATOM C	218	CE	LYS A 153	271.022	-49.981	97.450	1.00	62.23	A
	ATOM N	219	NZ	LYS A 153	272.289	-50.704	97.804	1.00	63.82	A
	ATOM C	220	C	LYS A 153	267.300	-48.233	93.056	1.00	60.69	A
10	ATOM O	221	O	LYS A 153	267.418	-47.029	93.188	1.00	68.16	A
	ATOM N	222	N	GLN A 154	266.890	-48.704	91.909	1.00	60.83	A
15	ATOM C	223	CA	GLN A 154	266.722	-47.630	90.954	1.00	60.63	A
	ATOM C	224	CB	GLN A 154	267.313	-48.015	89.612	1.00	65.34	A
	ATOM C	225	CG	GLN A 154	268.585	-48.908	89.762	1.00	73.31	A
20	ATOM C	226	CD	GLN A 154	268.842	-49.643	88.514	1.00	76.62	A
	ATOM O	227	OE1	GLN A 154	268.751	-49.059	87.368	1.00	77.22	A
25	ATOM N	228	NE2	GLN A 154	269.150	-50.963	88.658	1.00	79.75	A
	ATOM C	229	C	GLN A 154	265.288	-47.279	90.868	1.00	58.41	A
	ATOM O	230	O	GLN A 154	264.929	-46.135	90.760	1.00	66.80	A
30	ATOM N	231	N	SER A 155	264.465	-48.297	91.026	1.00	63.11	A
	ATOM C	232	CA	SER A 155	263.012	-48.182	90.986	1.00	57.08	A
	ATOM C	233	CB	SER A 155	262.438	-49.593	90.891	1.00	57.59	A
35	ATOM O	234	OG	SER A 155	261.096	-49.532	90.511	1.00	71.09	A
	ATOM C	235	C	SER A 155	262.393	-47.454	92.192	1.00	54.17	A
40	ATOM O	236	O	SER A 155	261.494	-46.653	92.054	1.00	41.48	A
	ATOM N	237	N	LYS A 156	262.919	-47.739	93.368	1.00	54.36	A
45	ATOM C	238	CA	LYS A 156	262.415	-47.187	94.614	1.00	65.54	A
	ATOM C	239	CB	LYS A 156	262.133	-45.687	94.476	1.00	68.88	A
	ATOM C	240	CG	LYS A 156	263.375	-44.809	94.527	1.00	68.98	A
50	ATOM C	241	CD	LYS A 156	263.018	-43.342	94.698	1.00	65.67	A
	ATOM C	242	CE	LYS A 156	262.170	-42.850	93.529	1.00	62.20	A
55	ATOM N	243	NZ	LYS A 156	261.774	-41.416	93.679	1.00	56.13	A
	ATOM C	244	C	LYS A 156	261.138	-47.958	95.009	1.00	64.77	A
	ATOM O	245	O	LYS A 156	260.317	-47.485	95.803	1.00	68.30	A
60	ATOM N	246	N	PHE A 157	261.012	-49.159	94.446	1.00	62.48	A
	ATOM C	247	CA	PHE A 157	259.891	-50.051	94.679	1.00	52.64	A

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5	ATOM C	279	CA	LEU A 161	262.564	-59.520	101.378	1.00	44.64	A
	ATOM C	280	CB	LEU A 161	263.916	-58.794	101.334	1.00	47.23	A
	ATOM C	281	CG	LEU A 161	264.865	-59.050	100.188	1.00	47.49	A
	ATOM C	282	CD1	LEU A 161	264.153	-58.846	98.870	1.00	42.04	A
10	ATOM C	283	CD2	LEU A 161	266.031	-58.125	100.309	1.00	46.85	A
	ATOM C	284	C	LEU A 161	262.607	-60.592	102.441	1.00	45.60	A
15	ATOM O	285	O	LEU A 161	263.013	-60.338	103.570	1.00	56.35	A
	ATOM N	286	N	LYS A 162	262.194	-61.801	102.078	1.00	46.81	A
	ATOM C	287	CA	LYS A 162	262.178	-62.940	103.009	1.00	41.78	A
20	ATOM C	288	CB	LYS A 162	261.104	-63.922	102.585	1.00	37.22	A
	ATOM C	289	CG	LYS A 162	260.826	-65.007	103.588	1.00	34.96	A
25	ATOM C	290	CD	LYS A 162	259.600	-65.804	103.219	1.00	30.75	A
	ATOM C	291	CE	LYS A 162	259.522	-67.056	104.081	1.00	32.45	A
	ATOM N	292	NZ	LYS A 162	258.194	-67.801	103.796	1.00	32.97	A
30	ATOM C	293	C	LYS A 162	263.521	-63.634	103.018	1.00	43.17	A
	ATOM O	294	O	LYS A 162	263.869	-64.350	102.087	1.00	50.65	A
35	ATOM N	295	N	VAL A 163	264.299	-63.369	104.049	1.00	47.41	A
	ATOM C	296	CA	VAL A 163	265.625	-63.965	104.187	1.00	50.56	A
	ATOM C	297	CB	VAL A 163	266.539	-63.091	105.120	1.00	49.49	A
40	ATOM C	298	CG1	VAL A 163	267.951	-63.664	105.180	1.00	43.15	A
	ATOM C	299	CG2	VAL A 163	266.555	-61.660	104.586	1.00	46.95	A
45	ATOM C	300	C	VAL A 163	265.570	-65.371	104.756	1.00	48.41	A
	ATOM O	301	O	VAL A 163	264.994	-65.586	105.798	1.00	53.08	A
	ATOM N	302	N	LEU A 164	266.195	-66.329	104.085	1.00	53.99	A
50	ATOM C	303	CA	LEU A 164	266.261	-67.732	104.569	1.00	55.36	A
	ATOM C	304	CB	LEU A 164	265.516	-68.657	103.598	1.00	54.99	A
55	ATOM C	305	CG	LEU A 164	264.173	-68.154	103.039	1.00	57.06	A
	ATOM C	306	CD1	LEU A 164	264.096	-68.423	101.535	1.00	57.49	A
	ATOM C	307	CD2	LEU A 164	263.093	-68.851	103.764	1.00	55.47	A
60	ATOM C	308	C	LEU A 164	267.715	-68.188	104.665	1.00	52.23	A
	ATOM O	309	O	LEU A 164	268.488	-67.990	103.745	1.00	50.98	A

5	ATOM N	310	N	PHE A 165	268.081	-68.800	105.774	1.00	52.15	A
	ATOM C	311	CA	PHE A 165	269.422	-69.297	105.892	1.00	51.87	A
	ATOM C	312	CB	PHE A 165	269.859	-69.322	107.352	1.00	54.79	A
	ATOM C	313	CG	PHE A 165	270.210	-67.979	107.875	1.00	59.43	A
10	ATOM C	314	CD1	PHE A 165	269.232	-67.171	108.426	1.00	61.03	A
	ATOM C	315	CD2	PHE A 165	271.517	-67.493	107.769	1.00	59.15	A
15	ATOM C	316	CE1	PHE A 165	269.542	-65.896	108.856	1.00	59.31	A
	ATOM C	317	CE2	PHE A 165	271.835	-66.216	108.196	1.00	59.42	A
20	ATOM C	318	CZ	PHE A 165	270.845	-65.412	108.745	1.00	60.41	A
	ATOM C	319	C	PHE A 165	269.598	-70.683	105.287	1.00	52.40	A
	ATOM O	320	O	PHE A 165	268.924	-71.654	105.675	1.00	45.64	A
25	ATOM N	321	N	LYS A 166	270.504	-70.772	104.320	1.00	52.32	A
	ATOM C	322	CA	LYS A 166	270.786	-72.050	103.696	1.00	53.94	A
	ATOM C	323	CB	LYS A 166	271.911	-71.916	102.708	1.00	47.98	A
30	ATOM C	324	CG	LYS A 166	271.540	-71.081	101.498	1.00	41.92	A
	ATOM C	325	CD	LYS A 166	272.530	-71.309	100.383	1.00	38.85	A
35	ATOM C	326	CE	LYS A 166	272.490	-70.201	99.345	1.00	31.90	A
	ATOM N	327	NZ	LYS A 166	273.477	-70.401	98.252	1.00	43.47	A
	ATOM C	328	C	LYS A 166	271.159	-73.067	104.740	1.00	51.94	A
40	ATOM O	329	O	LYS A 166	270.625	-74.147	104.743	1.00	62.20	A
	ATOM N	330	N	ALA A 167	272.031	-72.699	105.659	1.00	51.64	A
45	ATOM C	331	CA	ALA A 167	272.445	-73.632	106.682	1.00	51.81	A
	ATOM C	332	CB	ALA A 167	273.293	-72.935	107.670	1.00	53.31	A
	ATOM C	333	C	ALA A 167	271.234	-74.240	107.369	1.00	53.85	A
50	ATOM O	334	O	ALA A 167	271.105	-75.457	107.454	1.00	57.18	A
	ATOM N	335	N	GLN A 168	270.318	-73.403	107.833	1.00	59.28	A
55	ATOM C	336	CA	GLN A 168	269.139	-73.902	108.534	1.00	59.95	A
	ATOM C	337	CB	GLN A 168	268.348	-72.736	109.131	1.00	66.12	A
60	ATOM C	338	CG	GLN A 168	268.398	-72.648	110.644	1.00	72.61	A
	ATOM C	339	CD	GLN A 168	267.038	-72.270	111.248	1.00	77.64	A
	ATOM O	340	OE1	GLN A 168	266.542	-72.938	112.173	1.00	76.82	A

5	ATOM N	341	NE2	GLN A 168	266.432	-71.196	110.727	1.00	72.17	A
	ATOM C	342	C	GLN A 168	268.221	-74.718	107.635	1.00	55.73	A
	ATOM O	343	O	GLN A 168	267.646	-75.736	108.043	1.00	53.22	A
	ATOM N	344	N	LEU A 169	268.076	-74.262	106.404	1.00	47.44	A
10	ATOM C	345	CA	LEU A 169	267.214	-74.954	105.430	1.00	53.18	A
	ATOM C	346	CB	LEU A 169	267.236	-74.247	104.084	1.00	46.05	A
15	ATOM C	347	CG	LEU A 169	266.495	-72.939	104.055	1.00	47.35	A
	ATOM C	348	CD1	LEU A 169	266.858	-72.184	102.803	1.00	45.64	A
	ATOM C	349	CD2	LEU A 169	265.005	-73.224	104.130	1.00	44.94	A
20	ATOM C	350	C	LEU A 169	267.743	-76.381	105.180	1.00	53.79	A
	ATOM O	351	O	LEU A 169	266.983	-77.361	105.065	1.00	54.87	A
25	ATOM N	352	N	GLU A 170	269.057	-76.488	105.056	1.00	54.40	A
	ATOM C	353	CA	GLU A 170	269.692	-77.771	104.839	1.00	58.30	A
	ATOM C	354	CB	GLU A 170	271.162	-77.587	104.678	1.00	57.36	A
30	ATOM C	355	CG	GLU A 170	271.585	-77.158	103.319	1.00	66.04	A
	ATOM C	356	CD	GLU A 170	273.099	-76.836	103.260	1.00	73.19	A
35	ATOM O	357	OE1	GLU A 170	273.912	-77.755	103.560	1.00	76.86	A
	ATOM O	358	OE2	GLU A 170	273.473	-75.670	102.918	1.00	77.40	A
	ATOM C	359	C	GLU A 170	269.481	-78.643	106.045	1.00	60.58	A
40	ATOM O	360	O	GLU A 170	268.882	-79.730	105.913	1.00	71.27	A
	ATOM N	361	N	LYS A 171	269.931	-78.162	107.207	1.00	59.38	A
45	ATOM C	362	CA	LYS A 171	269.817	-78.942	108.423	1.00	59.74	A
	ATOM C	363	CB	LYS A 171	270.264	-78.118	109.600	1.00	58.50	A
50	ATOM C	364	C	LYS A 171	268.409	-79.500	108.655	1.00	62.87	A
	ATOM O	365	O	LYS A 171	268.227	-80.438	109.441	1.00	65.46	A
	ATOM N	366	N	ALA A 172	267.417	-78.939	107.970	1.00	58.04	A
55	ATOM C	367	CA	ALA A 172	266.044	-79.373	108.153	1.00	55.58	A
	ATOM C	368	CB	ALA A 172	265.139	-78.157	108.445	1.00	44.25	A
60	ATOM C	369	C	ALA A 172	265.506	-80.129	106.962	1.00	57.83	A
	ATOM O	370	O	ALA A 172	264.406	-80.699	107.038	1.00	63.97	A
	ATOM N	371	N	GLY A 173	266.255	-80.108	105.860	1.00	59.05	A

5	ATOM C	372	CA	GLY A 173	265.825	-80.806	104.659	1.00	58.57	A
	ATOM C	373	C	GLY A 173	264.519	-80.290	104.096	1.00	56.33	A
	ATOM O	374	O	GLY A 173	263.636	-81.045	103.722	1.00	57.22	A
	ATOM N	375	N	VAL A 174	264.392	-78.983	104.043	1.00	52.27	A
10	ATOM C	376	CA	VAL A 174	263.183	-78.389	103.520	1.00	51.67	A
	ATOM C	377	CB	VAL A 174	262.555	-77.420	104.523	1.00	44.57	A
15	ATOM C	378	CG1	VAL A 174	262.061	-78.172	105.687	1.00	45.83	A
	ATOM C	379	CG2	VAL A 174	263.557	-76.374	104.919	1.00	43.22	A
20	ATOM C	380	C	VAL A 174	263.518	-77.628	102.230	1.00	55.27	A
	ATOM O	381	O	VAL A 174	262.825	-76.679	101.851	1.00	62.81	A
	ATOM N	382	N	GLU A 175	264.577	-78.044	101.548	1.00	50.98	A
	ATOM C	383	CA	GLU A 175	264.955	-77.393	100.296	1.00	52.00	A
25	ATOM C	384	CB	GLU A 175	266.251	-77.994	99.721	1.00	47.79	A
	ATOM C	385	CG	GLU A 175	267.462	-77.861	100.680	1.00	59.64	A
30	ATOM C	386	CD	GLU A 175	267.730	-79.101	101.479	1.00	59.83	A
	ATOM O	387	OE1	GLU A 175	266.822	-79.948	101.619	1.00	66.12	A
35	ATOM O	388	OE2	GLU A 175	268.853	-79.219	101.990	1.00	70.43	A
	ATOM C	389	C	GLU A 175	263.852	-77.526	99.266	1.00	51.17	A
40	ATOM O	390	O	GLU A 175	263.637	-76.642	98.463	1.00	57.75	A
	ATOM N	391	N	HIS A 176	263.166	-78.661	99.266	1.00	60.20	A
	ATOM C	392	CA	HIS A 176	262.080	-78.920	98.312	1.00	61.34	A
45	ATOM C	393	CB	HIS A 176	261.735	-80.414	98.276	1.00	62.47	A
	ATOM C	394	CG	HIS A 176	261.265	-80.959	99.579	1.00	70.92	A
50	ATOM C	395	CD2	HIS A 176	261.875	-81.020	100.783	1.00	68.70	A
	ATOM N	396	ND1	HIS A 176	260.020	-81.533	99.740	1.00	72.07	A
	ATOM C	397	CE1	HIS A 176	259.886	-81.925	100.994	1.00	75.43	A
	ATOM N	398	NE2	HIS A 176	260.996	-81.625	101.644	1.00	77.22	A
55	ATOM C	399	C	HIS A 176	260.828	-78.116	98.620	1.00	60.76	A
	ATOM O	400	O	HIS A 176	260.058	-77.805	97.733	1.00	64.86	A
60	ATOM N	401	N	GLN A 177	260.607	-77.784	99.886	1.00	63.60	A
	ATOM C	402	CA	GLN A 177	259.436	-76.993	100.239	1.00	59.32	A

5	ATOM C	403	CB	GLN A 177	259.188	-77.080	101.756	1.00	65.79	A
	ATOM C	404	CG	GLN A 177	258.573	-78.484	102.090	1.00	78.25	A
	ATOM C	405	CD	GLN A 177	258.481	-78.896	103.539	1.00	84.93	A
	ATOM O	406	OE1	GLN A 177	257.670	-79.822	103.897	1.00	89.62	A
10	ATOM N	407	NE2	GLN A 177	259.316	-78.274	104.407	1.00	87.76	A
	ATOM C	408	C	GLN A 177	259.647	-75.552	99.730	1.00	54.25	A
15	ATOM O	409	O	GLN A 177	258.739	-75.013	99.073	1.00	51.39	A
	ATOM N	410	N	LEU A 178	260.844	-74.972	99.942	1.00	45.84	A
	ATOM C	411	CA	LEU A 178	261.123	-73.611	99.474	1.00	49.49	A
20	ATOM C	412	CB	LEU A 178	262.514	-73.175	99.900	1.00	42.21	A
	ATOM C	413	CG	LEU A 178	263.032	-71.858	99.325	1.00	49.26	A
25	ATOM C	414	CD1	LEU A 178	261.981	-70.693	99.584	1.00	37.20	A
	ATOM C	415	CD2	LEU A 178	264.421	-71.557	99.950	1.00	46.43	A
	ATOM C	416	C	LEU A 178	261.030	-73.631	97.939	1.00	46.87	A
30	ATOM O	417	O	LEU A 178	260.678	-72.659	97.280	1.00	52.87	A
	ATOM N	418	N	ARG A 179	261.314	-74.778	97.360	1.00	52.38	A
35	ATOM C	419	CA	ARG A 179	261.258	-74.887	95.908	1.00	48.78	A
	ATOM C	420	CB	ARG A 179	261.877	-76.207	95.443	1.00	55.74	A
	ATOM C	421	CG	ARG A 179	262.661	-76.085	94.149	1.00	55.19	A
40	ATOM C	422	CD	ARG A 179	263.898	-77.002	94.178	1.00	71.41	A
	ATOM N	423	NE	ARG A 179	264.829	-76.685	93.086	1.00	73.48	A
45	ATOM C	424	CZ	ARG A 179	264.827	-77.258	91.873	1.00	77.16	A
	ATOM N	425	NH1	ARG A 179	263.941	-78.208	91.565	1.00	70.26	A
	ATOM N	426	NH2	ARG A 179	265.709	-76.874	90.951	1.00	75.62	A
50	ATOM C	427	C	ARG A 179	259.841	-74.758	95.383	1.00	46.80	A
	ATOM O	428	O	ARG A 179	259.605	-74.009	94.443	1.00	37.96	A
55	ATOM N	429	N	ARG A 180	258.912	-75.494	95.988	1.00	41.56	A
	ATOM C	430	CA	ARG A 180	257.504	-75.451	95.630	1.00	46.45	A
	ATOM C	431	CB	ARG A 180	256.749	-76.543	96.386	1.00	47.01	A
60	ATOM C	432	CG	ARG A 180	256.416	-77.762	95.546	1.00	51.52	A
	ATOM C	433	CD	ARG A 180	255.582	-78.783	96.257	1.00	53.97	A

5	ATOM N	434	NE	ARG A 180	256.374	-79.863	96.824	1.00	69.57	A
	ATOM C	435	CZ	ARG A 180	256.902	-79.849	98.046	1.00	76.20	A
	ATOM N	436	NH1	ARG A 180	256.721	-78.796	98.846	1.00	85.82	A
	ATOM N	437	NH2	ARG A 180	257.614	-80.893	98.475	1.00	82.98	A
10	ATOM C	438	C	ARG A 180	256.882	-74.100	95.969	1.00	48.19	A
	ATOM O	439	O	ARG A 180	256.088	-73.556	95.189	1.00	55.26	A
15	ATOM N	440	N	GLU A 181	257.235	-73.560	97.130	1.00	49.77	A
	ATOM C	441	CA	GLU A 181	256.694	-72.279	97.536	1.00	48.24	A
	ATOM C	442	CB	GLU A 181	257.367	-71.820	98.841	1.00	51.28	A
20	ATOM C	443	CG	GLU A 181	256.969	-70.425	99.303	1.00	55.39	A
	ATOM C	444	CD	GLU A 181	257.553	-70.042	100.652	1.00	57.20	A
25	ATOM O	445	OE1	GLU A 181	258.173	-70.904	101.305	1.00	46.80	A
	ATOM O	446	OE2	GLU A 181	257.362	-68.871	101.058	1.00	56.40	A
	ATOM C	447	C	GLU A 181	256.958	-71.259	96.430	1.00	49.63	A
30	ATOM O	448	O	GLU A 181	256.044	-70.571	95.930	1.00	44.79	A
	ATOM N	449	N	VAL A 182	258.227	-71.191	96.037	1.00	46.11	A
35	ATOM C	450	CA	VAL A 182	258.659	-70.228	95.035	1.00	45.55	A
	ATOM C	451	CB	VAL A 182	260.183	-70.266	94.833	1.00	40.91	A
	ATOM C	452	CG1	VAL A 182	260.560	-69.403	93.678	1.00	38.12	A
40	ATOM C	453	CG2	VAL A 182	260.875	-69.730	96.059	1.00	51.08	A
	ATOM C	454	C	VAL A 182	257.954	-70.443	93.695	1.00	46.82	A
45	ATOM O	455	O	VAL A 182	257.459	-69.483	93.056	1.00	40.29	A
	ATOM N	456	N	GLU A 183	257.936	-71.690	93.237	1.00	48.08	A
	ATOM C	457	CA	GLU A 183	257.280	-72.012	91.968	1.00	52.62	A
50	ATOM C	458	CB	GLU A 183	257.493	-73.478	91.608	1.00	56.60	A
	ATOM C	459	CG	GLU A 183	258.695	-73.784	90.808	1.00	70.69	A
55	ATOM C	460	CD	GLU A 183	258.923	-75.283	90.746	1.00	77.34	A
	ATOM O	461	OE1	GLU A 183	257.954	-76.011	90.397	1.00	83.76	A
	ATOM O	462	OE2	GLU A 183	260.068	-75.727	91.052	1.00	82.45	A
60	ATOM C	463	C	GLU A 183	255.800	-71.754	91.912	1.00	49.85	A
	ATOM O	464	O	GLU A 183	255.313	-71.138	90.947	1.00	46.36	A

Line	Atom	Res	Chain	ResID	X	Y	Z	Occup	B-factor	Alt
5	ATOM N	465	N	ILE A 184	255.098	-72.317	92.898	1.00	46.74	A
	ATOM C	466	CA	ILE A 184	253.660	-72.157	92.965	1.00	43.86	A
	ATOM C	467	CB	ILE A 184	253.067	-72.962	94.115	1.00	40.26	A
	ATOM C	468	CG2	ILE A 184	251.553	-72.714	94.209	1.00	29.84	A
10	ATOM C	469	CG1	ILE A 184	253.313	-74.446	93.860	1.00	36.80	A
	ATOM C	470	CD1	ILE A 184	252.748	-75.369	94.961	1.00	40.80	A
	ATOM C	471	C	ILE A 184	253.221	-70.713	93.099	1.00	46.29	A
15	ATOM O	472	O	ILE A 184	252.448	-70.199	92.284	1.00	49.47	A
	ATOM N	473	N	GLN A 185	253.720	-70.054	94.132	1.00	49.28	A
20	ATOM C	474	CA	GLN A 185	253.328	-68.666	94.388	1.00	52.47	A
	ATOM C	475	CB	GLN A 185	253.948	-68.189	95.721	1.00	44.73	A
	ATOM C	476	CG	GLN A 185	253.150	-67.168	96.526	1.00	48.30	A
25	ATOM C	477	CD	GLN A 185	253.861	-66.745	97.745	1.00	54.47	A
	ATOM O	478	OE1	GLN A 185	254.700	-67.516	98.331	1.00	61.67	A
30	ATOM N	479	NE2	GLN A 185	253.553	-65.501	98.201	1.00	56.50	A
	ATOM C	480	C	GLN A 185	253.707	-67.716	93.231	1.00	50.63	A
	ATOM O	481	O	GLN A 185	252.971	-66.780	92.894	1.00	52.61	A
35	ATOM N	482	N	SER A 186	254.843	-67.972	92.610	1.00	47.27	A
	ATOM C	483	CA	SER A 186	255.315	-67.114	91.541	1.00	52.03	A
40	ATOM C	484	CB	SER A 186	256.692	-67.586	91.048	1.00	51.09	A
	ATOM O	485	OG	SER A 186	256.609	-68.877	90.496	1.00	54.11	A
	ATOM C	486	C	SER A 186	254.346	-67.050	90.373	1.00	51.30	A
45	ATOM O	487	O	SER A 186	254.116	-65.999	89.812	1.00	53.71	A
	ATOM N	488	N	HIS A 187	253.774	-68.184	90.001	1.00	55.86	A
50	ATOM C	489	CA	HIS A 187	252.846	-68.233	88.883	1.00	57.28	A
	ATOM C	490	CB	HIS A 187	252.945	-69.605	88.190	1.00	68.44	A
	ATOM C	491	CG	HIS A 187	254.283	-69.866	87.541	1.00	77.26	A
55	ATOM C	492	CD2	HIS A 187	255.147	-69.041	86.892	1.00	78.77	A
	ATOM N	493	ND1	HIS A 187	254.874	-71.114	87.532	1.00	80.45	A
60	ATOM C	494	CE1	HIS A 187	256.041	-71.048	86.911	1.00	81.91	A
	ATOM N	495	NE2	HIS A 187	256.232	-69.802	86.512	1.00	81.51	A

5	ATOM C	496	C	HIS A 187	251.418	-67.953	89.300	1.00	57.51	A
	ATOM O	497	O	HIS A 187	250.496	-68.154	88.529	1.00	60.26	A
	ATOM N	498	N	LEU A 188	251.230	-67.497	90.530	1.00	59.97	A
	ATOM C	499	CA	LEU A 188	249.900	-67.189	91.028	1.00	56.67	A
10	ATOM C	500	CB	LEU A 188	249.832	-67.488	92.511	1.00	57.07	A
	ATOM C	501	CG	LEU A 188	248.970	-68.663	92.952	1.00	55.73	A
15	ATOM C	502	CD1	LEU A 188	249.478	-69.896	92.257	1.00	62.61	A
	ATOM C	503	CD2	LEU A 188	249.027	-68.827	94.465	1.00	53.98	A
20	ATOM C	504	C	LEU A 188	249.598	-65.728	90.777	1.00	57.85	A
	ATOM O	505	O	LEU A 188	250.503	-64.881	90.799	1.00	64.49	A
	ATOM N	506	N	ARG A 189	248.331	-65.440	90.507	1.00	59.25	A
	ATOM C	507	CA	ARG A 189	247.893	-64.067	90.239	1.00	63.66	A
25	ATOM C	508	CB	ARG A 189	247.927	-63.796	88.734	1.00	64.78	A
	ATOM C	509	CG	ARG A 189	249.318	-63.660	88.125	1.00	70.33	A
30	ATOM C	510	CD	ARG A 189	249.903	-62.285	88.356	1.00	72.14	A
	ATOM N	511	NE	ARG A 189	250.864	-61.937	87.301	1.00	81.14	A
35	ATOM C	512	CZ	ARG A 189	250.716	-60.923	86.432	1.00	82.52	A
	ATOM N	513	NH1	ARG A 189	249.636	-60.138	86.478	1.00	79.99	A
	ATOM N	514	NH2	ARG A 189	251.658	-60.669	85.521	1.00	82.64	A
	ATOM C	515	C	ARG A 189	246.469	-63.844	90.761	1.00	59.43	A
40	ATOM O	516	O	ARG A 189	245.497	-64.167	90.072	1.00	61.20	A
	ATOM N	517	N	HIS A 190	246.342	-63.283	91.964	1.00	56.49	A
45	ATOM C	518	CA	HIS A 190	245.023	-63.075	92.565	1.00	48.34	A
	ATOM C	519	CB	HIS A 190	244.506	-64.377	93.201	1.00	52.70	A
50	ATOM C	520	CG	HIS A 190	243.036	-64.372	93.489	1.00	49.06	A
	ATOM C	521	CD2	HIS A 190	242.038	-65.207	93.107	1.00	52.53	A
55	ATOM N	522	ND1	HIS A 190	242.449	-63.432	94.302	1.00	51.06	A
	ATOM C	523	CE1	HIS A 190	241.155	-63.686	94.414	1.00	46.17	A
60	ATOM N	524	NE2	HIS A 190	240.878	-64.757	93.697	1.00	43.53	A
	ATOM C	525	C	HIS A 190	245.116	-61.998	93.611	1.00	47.54	A
	ATOM O	526	O	HIS A 190	246.077	-61.946	94.377	1.00	44.41	A

5	ATOM N	527	N	PRO A 191	244.119	-61.102	93.645	1.00	49.93	A
	ATOM C	528	CD	PRO A 191	242.947	-61.054	92.749	1.00	46.91	A
	ATOM C	529	CA	PRO A 191	244.070	-59.992	94.607	1.00	49.33	A
	ATOM C	530	CB	PRO A 191	242.694	-59.384	94.346	1.00	50.21	A
10	ATOM C	531	CG	PRO A 191	242.518	-59.644	92.887	1.00	48.82	A
	ATOM C	532	C	PRO A 191	244.239	-60.419	96.072	1.00	46.55	A
15	ATOM O	533	O	PRO A 191	244.892	-59.719	96.848	1.00	42.94	A
	ATOM N	534	N	ASN A 192	243.647	-61.555	96.434	1.00	42.75	A
	ATOM C	535	CA	ASN A 192	243.715	-62.060	97.791	1.00	48.46	A
20	ATOM C	536	CB	ASN A 192	242.378	-62.678	98.192	1.00	45.61	A
	ATOM C	537	CG	ASN A 192	241.206	-61.781	97.847	1.00	48.26	A
25	ATOM O	538	OD1	ASN A 192	240.715	-61.767	96.724	1.00	55.77	A
	ATOM N	539	ND2	ASN A 192	240.766	-61.020	98.804	1.00	48.89	A
	ATOM C	540	C	ASN A 192	244.831	-63.085	97.953	1.00	44.35	A
30	ATOM O	541	O	ASN A 192	244.725	-64.017	98.747	1.00	54.33	A
	ATOM N	542	N	ILE A 193	245.909	-62.901	97.204	1.00	42.87	A
35	ATOM C	543	CA	ILE A 193	247.067	-63.781	97.277	1.00	40.40	A
	ATOM C	544	CB	ILE A 193	247.054	-64.847	96.138	1.00	40.53	A
	ATOM C	545	CG2	ILE A 193	248.292	-65.733	96.243	1.00	22.41	A
40	ATOM C	546	CG1	ILE A 193	245.800	-65.732	96.274	1.00	36.30	A
	ATOM C	547	CD1	ILE A 193	245.709	-66.793	95.246	1.00	46.23	A
45	ATOM C	548	C	ILE A 193	248.330	-62.944	97.180	1.00	43.53	A
	ATOM O	549	O	ILE A 193	248.481	-62.176	96.228	1.00	41.20	A
	ATOM N	550	N	LEU A 194	249.217	-63.070	98.171	1.00	46.32	A
50	ATOM C	551	CA	LEU A 194	250.449	-62.307	98.168	1.00	48.93	A
	ATOM C	552	CB	LEU A 194	251.233	-62.511	99.477	1.00	44.51	A
55	ATOM C	553	CG	LEU A 194	252.485	-61.630	99.579	1.00	41.08	A
	ATOM C	554	CD1	LEU A 194	252.055	-60.195	99.956	1.00	43.64	A
	ATOM C	555	CD2	LEU A 194	253.437	-62.183	100.655	1.00	41.05	A
60	ATOM C	556	C	LEU A 194	251.290	-62.773	96.988	1.00	49.00	A
	ATOM O	557	O	LEU A 194	251.553	-63.975	96.826	1.00	53.77	A

	ATOM N	558	N	ARG	A	195	251.712	-61.823	96.162	1.00	43.08	A
	ATOM C	559	CA	ARG	A	195	252.553	-62.166	95.023	1.00	45.19	A
5	ATOM C	560	CB	ARG	A	195	252.509	-61.043	93.969	1.00	43.15	A
	ATOM C	561	CG	ARG	A	195	251.180	-60.913	93.213	1.00	46.56	A
10	ATOM C	562	CD	ARG	A	195	251.400	-60.798	91.730	1.00	59.57	A
	ATOM N	563	NE	ARG	A	195	252.816	-60.787	91.377	1.00	72.51	A
	ATOM C	564	CZ	ARG	A	195	253.288	-60.716	90.133	1.00	78.66	A
15	ATOM N	565	NH1	ARG	A	195	252.446	-60.646	89.119	1.00	80.03	A
	ATOM N	566	NH2	ARG	A	195	254.603	-60.723	89.898	1.00	82.29	A
20	ATOM C	567	C	ARG	A	195	254.004	-62.450	95.390	1.00	44.60	A
	ATOM O	568	O	ARG	A	195	254.470	-62.001	96.429	1.00	47.11	A
	ATOM N	569	N	LEU	A	196	254.710	-63.177	94.522	1.00	48.18	A
25	ATOM C	570	CA	LEU	A	196	256.116	-63.465	94.735	1.00	48.30	A
	ATOM C	571	CB	LEU	A	196	256.345	-64.954	95.048	1.00	50.39	A
30	ATOM C	572	CG	LEU	A	196	257.768	-65.343	95.383	1.00	41.45	A
	ATOM C	573	CD1	LEU	A	196	258.090	-64.804	96.698	1.00	58.09	A
	ATOM C	574	CD2	LEU	A	196	257.886	-66.788	95.411	1.00	44.21	A
35	ATOM C	575	C	LEU	A	196	256.799	-63.091	93.432	1.00	50.04	A
	ATOM O	576	O	LEU	A	196	256.887	-63.926	92.532	1.00	56.48	A
40	ATOM N	577	N	TYR	A	197	257.301	-61.854	93.359	1.00	52.17	A
	ATOM C	578	CA	TYR	A	197	257.970	-61.330	92.172	1.00	49.64	A
	ATOM C	579	CB	TYR	A	197	258.419	-59.908	92.460	1.00	44.72	A
45	ATOM C	580	CG	TYR	A	197	257.289	-59.034	92.959	1.00	43.03	A
	ATOM C	581	CD1	TYR	A	197	257.445	-58.246	94.117	1.00	44.46	A
50	ATOM C	582	CE1	TYR	A	197	256.439	-57.433	94.583	1.00	51.15	A
	ATOM C	583	CD2	TYR	A	197	256.085	-58.978	92.278	1.00	41.30	A
	ATOM C	584	CE2	TYR	A	197	255.057	-58.161	92.730	1.00	50.46	A
55	ATOM C	585	CZ	TYR	A	197	255.243	-57.390	93.887	1.00	52.65	A
	ATOM O	586	OH	TYR	A	197	254.234	-56.573	94.338	1.00	63.16	A
60	ATOM C	587	C	TYR	A	197	259.142	-62.186	91.684	1.00	51.16	A
	ATOM O	588	O	TYR	A	197	259.129	-62.683	90.572	1.00	58.21	A

	5	ATOM N	589	N	GLY A 198	260.141	-62.378	92.529	1.00	53.24	A
		ATOM C	590	CA	GLY A 198	261.296	-63.164	92.148	1.00	47.33	A
		ATOM C	591	C	GLY A 198	262.028	-63.697	93.360	1.00	48.93	A
		ATOM O	592	O	GLY A 198	261.447	-63.928	94.412	1.00	49.80	A
	10	ATOM N	593	N	TYR A 199	263.316	-63.941	93.204	1.00	48.77	A
		ATOM C	594	CA	TYR A 199	264.134	-64.436	94.315	1.00	50.98	A
		ATOM C	595	CB	TYR A 199	263.712	-65.834	94.699	1.00	54.11	A
	15	ATOM C	596	CG	TYR A 199	264.323	-66.921	93.853	1.00	56.57	A
		ATOM C	597	CD1	TYR A 199	265.506	-67.521	94.238	1.00	57.21	A
	20	ATOM C	598	CE1	TYR A 199	266.088	-68.526	93.471	1.00	58.18	A
		ATOM C	599	CD2	TYR A 199	263.715	-67.351	92.664	1.00	59.67	A
		ATOM C	600	CE2	TYR A 199	264.286	-68.349	91.899	1.00	59.17	A
	25	ATOM C	601	CZ	TYR A 199	265.479	-68.933	92.308	1.00	59.36	A
		ATOM O	602	OH	TYR A 199	266.075	-69.917	91.535	1.00	63.54	A
	30	ATOM C	603	C	TYR A 199	265.563	-64.463	93.826	1.00	48.41	A
		ATOM O	604	O	TYR A 199	265.787	-64.357	92.640	1.00	47.41	A
		ATOM N	605	N	<u>PHE A 200</u>	266.542	-64.591	94.701	1.00	43.25	A
	35	ATOM C	606	CA	PHE A 200	267.921	-64.582	94.221	1.00	40.67	A
		ATOM C	607	CB	PHE A 200	268.427	-63.159	93.950	1.00	43.34	A
	40	ATOM C	608	CG	PHE A 200	268.272	-62.218	95.134	1.00	48.79	A
		ATOM C	609	CD1	PHE A 200	269.249	-62.115	96.166	1.00	50.06	A
		ATOM C	610	CD2	PHE A 200	267.178	-61.322	95.162	1.00	52.88	A
	45	ATOM C	611	CE1	PHE A 200	269.107	-61.097	97.192	1.00	53.41	A
		ATOM C	612	CE2	PHE A 200	267.048	-60.331	96.166	1.00	49.85	A
	50	ATOM C	613	CZ	PHE A 200	267.993	-60.201	97.160	1.00	49.27	A
		ATOM C	614	C	PHE A 200	268.645	-65.113	95.325	1.00	47.09	A
		ATOM O	615	O	PHE A 200	268.037	-65.599	96.262	1.00	47.13	A
	55	ATOM N	616	N	HIS A 201	269.953	-65.125	95.219	1.00	56.46	A
		ATOM C	617	CA	HIS A 201	270.635	-65.604	96.382	1.00	56.94	A
	60	ATOM C	618	CB	HIS A 201	270.242	-67.052	96.679	1.00	62.89	A
		ATOM C	619	CG	HIS A 201	270.668	-68.030	95.648	1.00	66.27	A

	ATOM C	620	CD2	HIS A	201	270.131	-68.454	94.469	1.00	68.86	A
	ATOM N	621	ND1	HIS A	201	271.876	-68.658	95.778	1.00	70.42	A
5	ATOM C	622	CE1	HIS A	201	272.086	-69.425	94.727	1.00	63.77	A
	ATOM N	623	NE2	HIS A	201	271.048	-69.319	93.917	1.00	69.53	A
10	ATOM C	624	C	HIS A	201	272.082	-65.339	96.531	1.00	59.01	A
	ATOM O	625	O	HIS A	201	272.657	-64.604	95.737	1.00	56.46	A
	ATOM N	626	N	ASP A	202	272.636	-65.783	97.652	1.00	53.50	A
15	ATOM C	627	CA	ASP A	202	274.052	-65.546	97.850	1.00	58.12	A
	ATOM C	628	CB	ASP A	202	274.321	-64.225	98.617	1.00	61.13	A
20	ATOM C	629	CG	ASP A	202	273.888	-64.255	100.090	1.00	65.37	A
	ATOM O	630	OD1	ASP A	202	273.969	-65.308	100.803	1.00	69.09	A
	ATOM O	631	OD2	ASP A	202	273.489	-63.181	100.569	1.00	73.25	A
25	ATOM C	632	C	ASP A	202	274.782	-66.745	98.522	1.00	59.73	A
	ATOM O	633	O	ASP A	202	274.357	-67.899	98.426	1.00	61.93	A
30	ATOM N	634	N	ALA A	203	275.910	-66.473	99.163	1.00	59.60	A
	ATOM C	635	CA	ALA A	203	276.705	-67.507	99.793	1.00	59.87	A
	ATOM C	636	CB	ALA A	203	278.079	-66.933	100.191	1.00	57.31	A
35	ATOM C	637	C	ALA A	203	276.068	-68.138	100.990	1.00	60.08	A
	ATOM O	638	O	ALA A	203	276.287	-69.294	101.229	1.00	62.79	A
40	ATOM N	639	N	THR A	204	275.291	-67.377	101.748	1.00	60.13	A
	ATOM C	640	CA	THR A	204	274.700	-67.893	102.968	1.00	58.14	A
	ATOM C	641	CB	THR A	204	275.067	-67.010	104.168	1.00	54.92	A
45	ATOM O	642	OG1	THR A	204	275.068	-65.622	103.799	1.00	51.82	A
	ATOM C	643	CG2	THR A	204	276.406	-67.388	104.681	1.00	55.25	A
50	ATOM C	644	C	THR A	204	273.203	-68.070	102.993	1.00	61.74	A
	ATOM O	645	O	THR A	204	272.662	-69.063	103.547	1.00	66.23	A
55	ATOM N	646	N	ARG A	205	272.517	-67.099	102.434	1.00	58.56	A
	ATOM C	647	CA	ARG A	205	271.091	-67.217	102.444	1.00	58.96	A
	ATOM C	648	CB	ARG A	205	270.505	-66.287	103.493	1.00	56.07	A
60	ATOM C	649	CG	ARG A	205	270.986	-64.877	103.382	1.00	59.74	A
	ATOM C	650	CD	ARG A	205	271.764	-64.493	104.616	1.00	62.84	A

5	ATOM N	651	NE	ARG	A	205	272.739	-63.462	104.285	1.00	73.59	A
	ATOM C	652	CZ	ARG	A	205	273.407	-62.747	105.185	1.00	79.55	A
	ATOM N	653	NH1	ARG	A	205	273.198	-62.946	106.482	1.00	80.70	A
	ATOM N	654	NH2	ARG	A	205	274.297	-61.845	104.792	1.00	87.21	A
10	ATOM C	655	C	ARG	A	205	270.418	-67.012	101.120	1.00	56.37	A
	ATOM O	656	O	ARG	A	205	271.034	-66.604	100.116	1.00	64.50	A
15	ATOM N	657	N	VAL	A	206	269.150	-67.373	101.124	1.00	54.49	A
	ATOM C	658	CA	VAL	A	206	268.304	-67.238	99.960	1.00	50.29	A
20	ATOM C	659	CB	VAL	A	206	267.536	-68.522	99.670	1.00	47.01	A
	ATOM C	660	CG1	VAL	A	206	266.800	-68.370	98.374	1.00	38.39	A
	ATOM C	661	CG2	VAL	A	206	268.488	-69.696	99.620	1.00	42.93	A
	ATOM C	662	C	VAL	A	206	267.306	-66.124	100.321	1.00	50.23	A
25	ATOM O	663	O	VAL	A	206	266.870	-65.982	101.487	1.00	49.82	A
	ATOM N	664	N	TYR	A	207	266.958	-65.330	99.320	1.00	47.64	A
30	ATOM C	665	CA	TYR	A	207	266.053	-64.226	99.517	1.00	47.19	A
	ATOM C	666	CB	TYR	A	207	266.748	-62.879	99.204	1.00	44.49	A
35	ATOM C	667	CG	TYR	A	207	268.077	-62.684	99.852	1.00	52.24	A
	ATOM C	668	CD1	TYR	A	207	269.198	-63.362	99.385	1.00	51.97	A
	ATOM C	669	CE1	TYR	A	207	270.438	-63.194	99.978	1.00	60.89	A
	ATOM C	670	CD2	TYR	A	207	268.227	-61.820	100.938	1.00	55.49	A
40	ATOM C	671	CE2	TYR	A	207	269.499	-61.638	101.553	1.00	62.31	A
	ATOM C	672	CZ	TYR	A	207	270.583	-62.327	101.069	1.00	60.88	A
45	ATOM O	673	OH	TYR	A	207	271.783	-62.141	101.704	1.00	68.24	A
	ATOM C	674	C	TYR	A	207	264.837	-64.374	98.618	1.00	42.31	A
50	ATOM O	675	O	TYR	A	207	264.940	-64.704	97.438	1.00	43.03	A
	ATOM N	676	N	LEU	A	208	263.671	-64.078	99.171	1.00	47.18	A
55	ATOM C	677	CA	LEU	A	208	262.441	-64.129	98.377	1.00	49.66	A
	ATOM C	678	CB	LEU	A	208	261.411	-65.084	99.005	1.00	50.68	A
	ATOM C	679	CG	LEU	A	208	261.731	-66.573	98.967	1.00	50.97	A
60	ATOM C	680	CD1	LEU	A	208	260.525	-67.349	99.471	1.00	51.61	A
	ATOM C	681	CD2	LEU	A	208	262.019	-66.964	97.575	1.00	53.77	A

5	ATOM C	682	C	LEU A 208	261.849	-62.733	98.264	1.00	50.25	A
	ATOM O	683	O	LEU A 208	261.525	-62.085	99.278	1.00	54.78	A
10	ATOM N	684	N	ILE A 209	261.692	-62.286	97.027	1.00	50.37	A
	ATOM C	685	CA	ILE A 209	261.154	-60.971	96.752	1.00	49.74	A
15	ATOM C	686	CB	ILE A 209	261.695	-60.499	95.420	1.00	50.44	A
	ATOM C	687	CG2	ILE A 209	261.168	-59.096	95.082	1.00	50.97	A
20	ATOM C	688	CG1	ILE A 209	263.225	-60.485	95.511	1.00	49.66	A
	ATOM C	689	CD1	ILE A 209	263.919	-60.607	94.181	1.00	51.66	A
25	ATOM C	690	C	ILE A 209	259.624	-61.075	96.749	1.00	51.17	A
	ATOM O	691	O	ILE A 209	259.048	-61.543	95.755	1.00	54.45	A
30	ATOM N	692	N	LEU A 210	258.981	-60.655	97.854	1.00	47.03	A
	ATOM C	693	CA	LEU A 210	257.530	-60.728	97.990	1.00	43.40	A
35	ATOM C	694	CB	LEU A 210	257.164	-61.286	99.362	1.00	43.91	A
	ATOM C	695	CG	LEU A 210	257.762	-62.625	99.773	1.00	42.46	A
40	ATOM C	696	CD1	LEU A 210	257.695	-62.764	101.264	1.00	44.44	A
	ATOM C	697	CD2	LEU A 210	257.029	-63.701	99.100	1.00	44.23	A
45	ATOM C	698	C	LEU A 210	256.873	-59.393	97.827	1.00	42.69	A
	ATOM O	699	O	LEU A 210	257.528	-58.371	97.627	1.00	50.83	A
50	ATOM N	700	N	GLU A 211	255.552	-59.403	97.901	1.00	45.93	A
	ATOM C	701	CA	GLU A 211	254.757	-58.173	97.813	1.00	41.90	A
55	ATOM C	702	CB	GLU A 211	253.383	-58.471	97.201	1.00	39.85	A
	ATOM C	703	CG	GLU A 211	252.402	-57.354	97.290	1.00	41.17	A
60	ATOM C	704	CD	GLU A 211	250.976	-57.788	96.890	1.00	51.54	A
	ATOM O	705	OE1	GLU A 211	250.012	-56.980	97.025	1.00	57.54	A
65	ATOM O	706	OE2	GLU A 211	250.798	-58.950	96.438	1.00	52.59	A
	ATOM C	707	C	GLU A 211	254.608	-57.669	99.259	1.00	38.67	A
70	ATOM O	708	O	GLU A 211	254.507	-58.477	100.200	1.00	42.39	A
	ATOM N	709	N	TYR A 212	254.619	-56.346	99.428	1.00	43.63	A
75	ATOM C	710	CA	TYR A 212	254.500	-55.725	100.757	1.00	47.96	A
	ATOM C	711	CB	TYR A 212	255.181	-54.338	100.753	1.00	46.03	A
	ATOM C	712	CG	TYR A 212	255.029	-53.534	102.025	1.00	44.95	A

Residue	Atom	X	Y	Z	B	Occupancy	Alt Loc	Disorder	Occupancy	Alt Loc	Disorder
5	ATOM C	713	CD1	TYR A 212	255.255	-54.104	103.259	1.00	42.54		A
	ATOM C	714	CE1	TYR A 212	255.084	-53.363	104.429	1.00	48.54		A
	ATOM C	715	CD2	TYR A 212	254.639	-52.193	101.984	1.00	44.86		A
	ATOM C	716	CE2	TYR A 212	254.473	-51.424	103.164	1.00	50.04		A
10	ATOM C	717	CZ	TYR A 212	254.693	-52.019	104.372	1.00	48.45		A
	ATOM O	718	OH	TYR A 212	254.523	-51.276	105.514	1.00	53.45		A
15	ATOM C	719	C	TYR A 212	253.041	-55.618	101.248	1.00	50.57		A
	ATOM O	720	O	TYR A 212	252.153	-55.140	100.508	1.00	51.02		A
	ATOM N	721	N	ALA A 213	252.799	-56.105	102.475	1.00	48.23		A
20	ATOM C	722	CA	ALA A 213	251.459	-56.040	103.078	1.00	51.96		A
	ATOM C	723	CB	ALA A 213	251.084	-57.386	103.656	1.00	42.77		A
25	ATOM C	724	C	ALA A 213	251.528	-54.973	104.177	1.00	46.25		A
	ATOM O	725	O	ALA A 213	251.958	-55.259	105.280	1.00	57.39		A
	ATOM N	726	N	PRO A 214	251.109	-53.734	103.869	1.00	45.44		A
30	ATOM C	727	CD	PRO A 214	250.592	-53.315	102.549	1.00	45.81		A
	ATOM C	728	CA	PRO A 214	251.118	-52.597	104.782	1.00	37.64		A
35	ATOM C	729	CB	PRO A 214	250.400	-51.512	103.991	1.00	44.41		A
	ATOM C	730	CG	PRO A 214	250.755	-51.821	102.584	1.00	45.51		A
	ATOM C	731	C	PRO A 214	250.481	-52.833	106.112	1.00	39.63		A
40	ATOM O	732	O	PRO A 214	251.116	-52.486	107.123	1.00	38.67		A
	ATOM N	733	N	LEU A 215	249.287	-53.446	106.124	1.00	33.01		A
45	ATOM C	734	CA	LEU A 215	248.570	-53.617	107.371	1.00	35.54		A
	ATOM C	735	CB	LEU A 215	247.074	-53.585	107.083	1.00	39.80		A
	ATOM C	736	CG	LEU A 215	246.571	-52.332	106.331	1.00	39.22		A
50	ATOM C	737	CD1	LEU A 215	245.025	-52.236	106.407	1.00	37.56		A
	ATOM C	738	CD2	LEU A 215	247.156	-51.166	106.898	1.00	36.39		A
55	ATOM C	739	C	LEU A 215	248.923	-54.805	108.248	1.00	43.21		A
	ATOM O	740	O	LEU A 215	248.208	-55.121	109.220	1.00	39.03		A
	ATOM N	741	N	GLY A 216	250.022	-55.466	107.906	1.00	42.62		A
60	ATOM C	742	CA	GLY A 216	250.443	-56.630	108.669	1.00	46.42		A
	ATOM C	743	C	GLY A 216	249.594	-57.891	108.554	1.00	44.15		A

Residue	Atom	Res	Chain	Seq	X	Y	Z	Occup	B-factor	Alt
5	ATOM O	744	O	GLY A 216	248.995	-58.166	107.504	1.00	46.45	A
	ATOM N	745	N	THR A 217	249.523	-58.640	109.656	1.00	39.98	A
	ATOM C	746	CA	THR A 217	248.774	-59.889	109.669	1.00	43.21	A
	ATOM C	747	CB	THR A 217	249.583	-61.040	110.286	1.00	43.67	A
10	ATOM O	748	OG1	THR A 217	249.791	-60.782	111.678	1.00	51.00	A
	ATOM C	749	CG2	THR A 217	250.905	-61.201	109.605	1.00	41.04	A
15	ATOM C	750	C	THR A 217	247.450	-59.858	110.416	1.00	42.99	A
	ATOM O	751	O	THR A 217	247.185	-58.962	111.227	1.00	41.59	A
20	ATOM N	752	N	VAL A 218	246.646	-60.881	110.166	1.00	41.73	A
	ATOM C	753	CA	VAL A 218	245.335	-61.037	110.766	1.00	41.12	A
	ATOM C	754	CB	VAL A 218	244.564	-62.091	109.970	1.00	41.84	A
	ATOM C	755	CG1	VAL A 218	243.170	-62.251	110.488	1.00	43.61	A
25	ATOM C	756	CG2	VAL A 218	244.544	-61.670	108.463	1.00	33.71	A
	ATOM C	757	C	VAL A 218	245.610	-61.486	112.201	1.00	40.94	A
30	ATOM O	758	O	VAL A 218	244.789	-61.326	113.078	1.00	51.00	A
	ATOM N	759	N	TYR A 219	246.801	-62.026	112.429	1.00	45.88	A
35	ATOM C	760	CA	TYR A 219	247.233	-62.484	113.757	1.00	42.54	A
	ATOM C	761	CB	TYR A 219	248.607	-63.148	113.673	1.00	45.91	A
	ATOM C	762	CG	TYR A 219	249.102	-63.676	115.011	1.00	46.80	A
	ATOM C	763	CD1	TYR A 219	248.755	-64.925	115.464	1.00	45.83	A
40	ATOM C	764	CE1	TYR A 219	249.176	-65.377	116.693	1.00	53.23	A
	ATOM C	765	CD2	TYR A 219	249.884	-62.892	115.825	1.00	46.38	A
45	ATOM C	766	CE2	TYR A 219	250.310	-63.314	117.053	1.00	52.61	A
	ATOM C	767	CZ	TYR A 219	249.961	-64.565	117.510	1.00	53.76	A
50	ATOM O	768	OH	TYR A 219	250.361	-64.985	118.789	1.00	54.10	A
	ATOM C	769	C	TYR A 219	247.323	-61.287	114.702	1.00	44.93	A
55	ATOM O	770	O	TYR A 219	246.745	-61.322	115.825	1.00	40.09	A
	ATOM N	771	N	ARG A 220	248.031	-60.243	114.240	1.00	37.14	A
60	ATOM C	772	CA	ARG A 220	248.172	-59.035	115.029	1.00	44.63	A
	ATOM C	773	CB	ARG A 220	249.213	-58.086	114.396	1.00	42.95	A
	ATOM C	774	C	ARG A 220	246.828	-58.318	115.225	1.00	43.95	A

5	ATOM O	775	O	ARG A 220	246.563	-57.773	116.314	1.00	44.55	A
	ATOM N	776	N	GLU A 221	245.973	-58.369	114.198	1.00	44.85	A
	ATOM C	777	CA	GLU A 221	244.688	-57.692	114.255	1.00	43.30	A
	ATOM C	778	CB	GLU A 221	244.031	-57.678	112.884	1.00	46.86	A
10	ATOM C	779	CG	GLU A 221	242.921	-56.648	112.713	1.00	56.65	A
	ATOM C	780	CD	GLU A 221	243.442	-55.193	112.758	1.00	63.09	A
15	ATOM O	781	OE1	GLU A 221	242.629	-54.238	112.637	1.00	66.10	A
	ATOM O	782	OE2	GLU A 221	244.670	-55.005	112.919	1.00	66.07	A
	ATOM C	783	C	GLU A 221	243.806	-58.412	115.243	1.00	46.56	A
20	ATOM O	784	O	GLU A 221	242.959	-57.802	115.900	1.00	44.66	A
	ATOM N	785	N	LEU A 222	244.028	-59.719	115.362	1.00	46.74	A
25	ATOM C	786	CA	LEU A 222	243.259	-60.550	116.272	1.00	40.98	A
	ATOM C	787	CB	LEU A 222	243.444	-62.013	115.880	1.00	42.79	A
	ATOM C	788	CG	LEU A 222	242.339	-62.985	116.313	1.00	48.20	A
30	ATOM C	789	CD1	LEU A 222	240.982	-62.509	115.826	1.00	42.35	A
	ATOM C	790	CD2	LEU A 222	242.649	-64.361	115.761	1.00	47.96	A
35	ATOM C	791	C	LEU A 222	243.744	-60.292	117.718	1.00	45.64	A
	ATOM O	792	O	LEU A 222	242.995	-60.390	118.692	1.00	46.35	A
	ATOM N	793	N	GLN A 223	245.008	-59.938	117.875	1.00	47.19	A
40	ATOM C	794	CA	GLN A 223	245.539	-59.670	119.203	1.00	48.16	A
	ATOM C	795	CB	GLN A 223	247.056	-59.584	119.112	1.00	49.22	A
45	ATOM C	796	CG	GLN A 223	247.819	-60.926	119.032	1.00	56.96	A
	ATOM C	797	CD	GLN A 223	249.300	-60.732	118.879	1.00	66.12	A
	ATOM O	798	OE1	GLN A 223	249.807	-59.935	117.981	1.00	68.93	A
50	ATOM N	799	NE2	GLN A 223	250.067	-61.453	119.755	1.00	65.96	A
	ATOM C	800	C	GLN A 223	244.994	-58.332	119.711	1.00	54.79	A
55	ATOM O	801	O	GLN A 223	244.710	-58.153	120.899	1.00	63.31	A
	ATOM N	802	N	LYS A 224	244.877	-57.398	118.779	1.00	53.43	A
60	ATOM C	803	CA	LYS A 224	244.412	-56.042	119.021	1.00	52.16	A
	ATOM C	804	CB	LYS A 224	244.668	-55.276	117.729	1.00	51.41	A
	ATOM C	805	CG	LYS A 224	244.740	-53.805	117.796	1.00	58.82	A

5	ATOM C	806	CD	LYS A 224	245.109	-53.234	116.429	1.00	58.34	A
	ATOM C	807	CE	LYS A 224	244.105	-52.175	115.957	1.00	57.11	A
	ATOM N	808	NZ	LYS A 224	243.509	-52.549	114.632	1.00	62.05	A
	ATOM C	809	C	LYS A 224	242.909	-55.999	119.415	1.00	46.25	A
10	ATOM O	810	O	LYS A 224	242.551	-55.374	120.392	1.00	53.53	A
	ATOM N	811	N	LEU A 225	242.054	-56.685	118.658	1.00	40.03	A
15	ATOM C	812	CA	LEU A 225	240.616	-56.712	118.885	1.00	28.18	A
	ATOM C	813	CB	LEU A 225	239.918	-56.682	117.544	1.00	32.03	A
	ATOM C	814	CG	LEU A 225	240.538	-55.704	116.515	1.00	37.72	A
20	ATOM C	815	CD1	LEU A 225	239.725	-55.736	115.208	1.00	28.64	A
	ATOM C	816	CD2	LEU A 225	240.577	-54.252	117.096	1.00	32.47	A
25	ATOM C	817	C	LEU A 225	240.076	-57.907	119.686	1.00	39.70	A
	ATOM O	818	O	LEU A 225	238.896	-57.954	120.056	1.00	27.45	A
	ATOM N	819	N	SER A 226	240.939	-58.877	119.958	1.00	33.23	A
30	ATOM C	820	CA	SER A 226	240.528	-60.051	120.695	1.00	38.91	A
	ATOM C	821	CB	SER A 226	239.864	-59.653	122.015	1.00	42.93	A
35	ATOM O	822	OG	SER A 226	240.536	-58.570	122.642	1.00	59.01	A
	ATOM C	823	C	SER A 226	239.548	-60.869	119.867	1.00	40.96	A
	ATOM O	824	O	SER A 226	239.777	-62.029	119.592	1.00	45.01	A
40	ATOM N	825	N	LYS A 227	238.433	-60.270	119.484	1.00	43.12	A
	ATOM C	826	CA	LYS A 227	237.409	-60.968	118.693	1.00	37.87	A
45	ATOM C	827	CB	LYS A 227	236.160	-61.246	119.551	1.00	41.34	A
	ATOM C	828	CG	LYS A 227	236.384	-62.150	120.650	1.00	49.95	A
	ATOM C	829	CD	LYS A 227	235.126	-62.365	121.469	1.00	59.51	A
50	ATOM C	830	CE	LYS A 227	234.854	-61.186	122.468	1.00	64.97	A
	ATOM N	831	NZ	LYS A 227	234.813	-61.628	123.907	1.00	64.50	A
55	ATOM C	832	C	LYS A 227	237.009	-60.044	117.520	1.00	37.96	A
	ATOM O	833	O	LYS A 227	237.061	-58.799	117.619	1.00	40.95	A
60	ATOM N	834	N	PHE A 228	236.575	-60.655	116.431	1.00	34.94	A
	ATOM C	835	CA	PHE A 228	236.175	-59.917	115.262	1.00	34.74	A
	ATOM C	836	CB	PHE A 228	236.793	-60.534	113.998	1.00	34.85	A

Atom	Res	Chain	Atom	X	Y	Z	Occupancy	B-factor	Alt
ATOM C	837	CG	PHE A 228	238.248	-60.293	113.849	1.00	43.10	A
ATOM C	838	CD1	PHE A 228	238.975	-61.009	112.913	1.00	43.37	A
ATOM C	839	CD2	PHE A 228	238.899	-59.395	114.656	1.00	38.38	A
ATOM C	840	CE1	PHE A 228	240.341	-60.832	112.796	1.00	48.51	A
ATOM C	841	CE2	PHE A 228	240.266	-59.207	114.554	1.00	47.20	A
ATOM C	842	CZ	PHE A 228	240.999	-59.919	113.631	1.00	48.16	A
ATOM C	843	C	PHE A 228	234.654	-60.063	115.208	1.00	40.38	A
ATOM O	844	O	PHE A 228	234.102	-61.082	115.664	1.00	36.38	A
ATOM N	845	N	ASP A 229	233.963	-59.053	114.687	1.00	40.55	A
ATOM C	846	CA	ASP A 229	232.525	-59.184	114.534	1.00	38.86	A
ATOM C	847	CB	ASP A 229	231.823	-57.832	114.440	1.00	49.26	A
ATOM C	848	CG	ASP A 229	232.394	-56.912	113.357	1.00	51.97	A
ATOM O	849	OD1	ASP A 229	232.396	-57.278	112.179	1.00	54.02	A
ATOM O	850	OD2	ASP A 229	232.806	-55.788	113.699	1.00	55.60	A
ATOM C	851	C	ASP A 229	232.180	-60.027	113.304	1.00	41.70	A
ATOM O	852	O	ASP A 229	233.039	-60.366	112.480	1.00	35.62	A
ATOM N	853	N	GLU A 230	230.905	-60.365	113.193	1.00	40.43	A
ATOM C	854	CA	GLU A 230	230.434	-61.213	112.114	1.00	43.61	A
ATOM C	855	CB	GLU A 230	228.939	-61.526	112.298	1.00	43.33	A
ATOM C	856	CG	GLU A 230	228.630	-62.147	113.653	1.00	43.90	A
ATOM C	857	CD	GLU A 230	227.292	-62.967	113.627	1.00	48.51	A
ATOM O	858	OE1	GLU A 230	226.230	-62.374	113.308	1.00	37.93	A
ATOM O	859	OE2	GLU A 230	227.300	-64.204	113.916	1.00	42.11	A
ATOM C	860	C	GLU A 230	230.661	-60.546	110.778	1.00	43.16	A
ATOM O	861	O	GLU A 230	230.878	-61.205	109.779	1.00	50.29	A
ATOM N	862	N	GLN A 231	230.590	-59.225	110.748	1.00	49.18	A
ATOM C	863	CA	GLN A 231	230.742	-58.501	109.489	1.00	49.70	A
ATOM C	864	CB	GLN A 231	230.311	-57.029	109.685	1.00	57.14	A
ATOM C	865	CG	GLN A 231	229.958	-56.236	108.412	1.00	62.54	A
ATOM C	866	CD	GLN A 231	231.200	-55.770	107.642	1.00	71.69	A
ATOM O	867	OE1	GLN A 231	232.065	-55.042	108.191	1.00	72.68	A

Residue	Atom	Res	Chain	Seq	X	Y	Z	Occupancy	B-factor	Alt. Loc.	Occupancy
5	ATOM N	868	NE2	GLN A 231	231.300	-56.184	106.359	1.00	72.33		A
	ATOM C	869	C	GLN A 231	232.197	-58.614	109.018	1.00	45.76		A
	ATOM O	870	O	GLN A 231	232.470	-58.874	107.846	1.00	46.46		A
	ATOM N	871	N	ARG A 232	233.131	-58.437	109.949	1.00	43.95		A
10	ATOM C	872	CA	ARG A 232	234.560	-58.503	109.661	1.00	38.33		A
	ATOM C	873	CB	ARG A 232	235.365	-57.998	110.861	1.00	39.16		A
15	ATOM C	874	CG	ARG A 232	236.867	-58.073	110.703	1.00	31.46		A
	ATOM C	875	CD	ARG A 232	237.514	-57.172	111.705	1.00	51.25		A
20	ATOM N	876	NE	ARG A 232	238.871	-56.815	111.334	1.00	58.24		A
	ATOM C	877	CZ	ARG A 232	239.275	-55.581	111.111	1.00	65.45		A
	ATOM N	878	NH1	ARG A 232	238.395	-54.594	111.226	1.00	62.94		A
	ATOM N	879	NH2	ARG A 232	240.551	-55.369	110.780	1.00	72.17		A
25	ATOM C	880	C	ARG A 232	234.950	-59.946	109.369	1.00	42.02		A
	ATOM O	881	O	ARG A 232	235.757	-60.183	108.517	1.00	45.04		A
30	ATOM N	882	N	THR A 233	234.372	-60.909	110.084	1.00	43.50		A
	ATOM C	883	CA	THR A 233	234.697	-62.320	109.891	1.00	37.00		A
35	ATOM C	884	CB	THR A 233	234.104	-63.175	110.992	1.00	35.89		A
	ATOM O	885	OG1	THR A 233	234.543	-62.696	112.268	1.00	30.74		A
40	ATOM C	886	CG2	THR A 233	234.488	-64.641	110.763	1.00	22.73		A
	ATOM C	887	C	THR A 233	234.149	-62.834	108.555	1.00	45.73		A
45	ATOM O	888	O	THR A 233	234.857	-63.523	107.844	1.00	45.99		A
	ATOM N	889	N	ALA A 234	232.892	-62.501	108.228	1.00	44.83		A
	ATOM C	890	CA	ALA A 234	232.256	-62.897	106.960	1.00	41.77		A
	ATOM C	891	CB	ALA A 234	230.852	-62.351	106.893	1.00	39.48		A
50	ATOM C	892	C	ALA A 234	233.064	-62.395	105.744	1.00	44.77		A
	ATOM O	893	O	ALA A 234	233.273	-63.131	104.786	1.00	39.69		A
55	ATOM N	894	N	THR A 235	233.543	-61.155	105.799	1.00	43.07		A
	ATOM C	895	CA	THR A 235	234.328	-60.579	104.722	1.00	44.31		A
60	ATOM C	896	CB	THR A 235	234.557	-59.058	104.926	1.00	44.88		A
	ATOM O	897	OG1	THR A 235	233.306	-58.373	104.984	1.00	49.29		A
	ATOM C	898	CG2	THR A 235	235.343	-58.498	103.807	1.00	37.93		A

[illegible]

5	ATOM C	930	CB	GLU A 239	238.937	-61.932	101.203	1.00	54.22	A
	ATOM C	931	CG	GLU A 239	238.139	-60.624	101.260	1.00	55.95	A
	ATOM C	932	CD	GLU A 239	238.811	-59.573	102.137	1.00	58.38	A
	ATOM O	933	OE1	GLU A 239	239.056	-59.843	103.333	1.00	65.65	A
10	ATOM O	934	OE2	GLU A 239	239.099	-58.468	101.634	1.00	60.73	A
	ATOM C	935	C	GLU A 239	239.109	-64.330	100.496	1.00	50.02	A
15	ATOM O	936	O	GLU A 239	239.851	-64.616	99.561	1.00	55.72	A
	ATOM N	937	N	LEU A 240	238.978	-65.104	101.557	1.00	49.14	A
20	ATOM C	938	CA	LEU A 240	239.768	-66.305	101.702	1.00	48.27	A
	ATOM C	939	CB	LEU A 240	239.776	-66.717	103.173	1.00	46.82	A
	ATOM C	940	CG	LEU A 240	240.917	-67.581	103.679	1.00	45.79	A
25	ATOM C	941	CD1	LEU A 240	242.225	-67.030	103.195	1.00	50.28	A
	ATOM C	942	CD2	LEU A 240	240.885	-67.603	105.172	1.00	53.83	A
30	ATOM C	943	C	LEU A 240	239.209	-67.420	100.833	1.00	49.65	A
	ATOM O	944	O	LEU A 240	239.960	-68.170	100.210	1.00	53.66	A
	ATOM N	945	N	ALA A 241	237.883	-67.519	100.778	1.00	45.02	A
35	ATOM C	946	CA	ALA A 241	237.222	-68.549	99.965	1.00	50.04	A
	ATOM C	947	CB	ALA A 241	235.724	-68.611	100.256	1.00	39.53	A
40	ATOM C	948	C	ALA A 241	237.447	-68.278	98.481	1.00	47.71	A
	ATOM O	949	O	ALA A 241	237.495	-69.203	97.682	1.00	54.94	A
	ATOM N	950	N	ASN A 242	237.585	-67.012	98.114	1.00	49.50	A
45	ATOM C	951	CA	ASN A 242	237.839	-66.637	96.729	1.00	51.78	A
	ATOM C	952	CB	ASN A 242	237.688	-65.134	96.554	1.00	45.48	A
50	ATOM C	953	CG	ASN A 242	236.231	-64.680	96.592	1.00	51.39	A
	ATOM O	954	OD1	ASN A 242	235.972	-63.489	96.769	1.00	50.23	A
	ATOM N	955	ND2	ASN A 242	235.276	-65.620	96.412	1.00	43.58	A
55	ATOM C	956	C	ASN A 242	239.241	-67.046	96.330	1.00	50.85	A
	ATOM O	957	O	ASN A 242	239.419	-67.736	95.323	1.00	53.87	A
60	ATOM N	958	N	ALA A 243	240.230	-66.625	97.119	1.00	48.27	A
	ATOM C	959	CA	ALA A 243	241.629	-66.970	96.861	1.00	42.21	A
	ATOM C	960	CB	ALA A 243	242.534	-66.345	97.913	1.00	45.13	A

5	ATOM C	961	C	ALA A 243	241.816	-68.473	96.880	1.00	43.95	A
	ATOM O	962	O	ALA A 243	242.498	-69.016	96.026	1.00	42.43	A
	ATOM N	963	N	LEU A 244	241.219	-69.152	97.858	1.00	40.59	A
	ATOM C	964	CA	LEU A 244	241.366	-70.606	97.945	1.00	48.68	A
10	ATOM C	965	CB	LEU A 244	240.689	-71.141	99.204	1.00	42.37	A
	ATOM C	966	CG	LEU A 244	241.465	-70.944	100.495	1.00	39.60	A
15	ATOM C	967	CD1	LEU A 244	240.751	-71.763	101.602	1.00	37.99	A
	ATOM C	968	CD2	LEU A 244	242.889	-71.432	100.340	1.00	35.22	A
20	ATOM C	969	C	LEU A 244	240.779	-71.311	96.702	1.00	56.87	A
	ATOM O	970	O	LEU A 244	241.327	-72.330	96.220	1.00	60.52	A
	ATOM N	971	N	SER A 245	239.662	-70.777	96.200	1.00	61.51	A
	ATOM C	972	CA	SER A 245	239.010	-71.317	95.018	1.00	61.35	A
25	ATOM C	973	CB	SER A 245	237.785	-70.501	94.692	1.00	64.64	A
	ATOM O	974	OG	SER A 245	237.339	-70.779	93.390	1.00	71.14	A
30	ATOM C	975	C	SER A 245	239.981	-71.242	93.855	1.00	63.54	A
	ATOM O	976	O	SER A 245	240.179	-72.233	93.134	1.00	63.37	A
35	ATOM N	977	N	TYR A 246	240.581	-70.063	93.679	1.00	58.29	A
	ATOM C	978	CA	TYR A 246	241.571	-69.855	92.633	1.00	57.08	A
	ATOM C	979	CB	TYR A 246	242.123	-68.455	92.719	1.00	51.38	A
40	ATOM C	980	CG	TYR A 246	243.247	-68.195	91.754	1.00	55.36	A
	ATOM C	981	CD1	TYR A 246	242.994	-67.652	90.492	1.00	50.94	A
45	ATOM C	982	CE1	TYR A 246	244.042	-67.382	89.609	1.00	55.86	A
	ATOM C	983	CD2	TYR A 246	244.584	-68.473	92.111	1.00	54.39	A
	ATOM C	984	CE2	TYR A 246	245.650	-68.213	91.234	1.00	55.81	A
50	ATOM C	985	CZ	TYR A 246	245.372	-67.665	89.982	1.00	55.07	A
	ATOM O	986	OH	TYR A 246	246.409	-67.409	89.112	1.00	55.05	A
55	ATOM C	987	C	TYR A 246	242.732	-70.852	92.733	1.00	57.54	A
	ATOM O	988	O	TYR A 246	243.234	-71.322	91.718	1.00	64.40	A
	ATOM N	989	N	CYS A 247	243.150	-71.180	93.951	1.00	56.76	A
60	ATOM C	990	CA	CYS A 247	244.245	-72.120	94.148	1.00	57.81	A
	ATOM C	991	CB	CYS A 247	244.779	-72.066	95.599	1.00	52.55	A

	ATOM S	992	SG	CYS A 247	245.687	-70.569	96.004	1.00	57.32	A
	ATOM C	993	C	CYS A 247	243.813	-73.538	93.837	1.00	59.03	A
5	ATOM O	994	O	CYS A 247	244.535	-74.272	93.143	1.00	61.55	A
	ATOM N	995	N	HIS A 248	242.659	-73.930	94.374	1.00	60.08	A
10	ATOM C	996	CA	HIS A 248	242.151	-75.291	94.156	1.00	58.63	A
	ATOM C	997	CB	HIS A 248	240.916	-75.540	95.036	1.00	57.40	A
	ATOM C	998	CG	HIS A 248	241.217	-75.606	96.496	1.00	54.60	A
15	ATOM C	999	CD2	HIS A 248	242.393	-75.694	97.160	1.00	54.55	A
	ATOM N	1000	ND1	HIS A 248	240.231	-75.623	97.459	1.00	54.23	A
20	ATOM C	1001	CE1	HIS A 248	240.789	-75.721	98.654	1.00	51.97	A
	ATOM N	1002	NE2	HIS A 248	242.099	-75.765	98.501	1.00	50.58	A
	ATOM C	1003	C	HIS A 248	241.806	-75.535	92.668	1.00	58.67	A
25	ATOM O	1004	O	HIS A 248	241.857	-76.667	92.171	1.00	50.45	A
	ATOM N	1005	N	SER A 249	241.459	-74.464	91.959	1.00	53.97	A
30	ATOM C	1006	CA	SER A 249	241.133	-74.589	90.550	1.00	58.32	A
	ATOM C	1007	CB	SER A 249	240.647	-73.248	89.991	1.00	55.40	A
	ATOM O	1008	OG	SER A 249	241.757	-72.480	89.526	1.00	54.94	A
35	ATOM C	1009	C	SER A 249	242.407	-75.020	89.798	1.00	58.15	A
	ATOM O	1010	O	SER A 249	242.326	-75.573	88.707	1.00	70.94	A
40	ATOM N	1011	N	LYS A 250	243.574	-74.746	90.370	1.00	51.49	A
	ATOM C	1012	CA	LYS A 250	244.820	-75.119	89.753	1.00	46.67	A
	ATOM C	1013	CB	LYS A 250	245.818	-73.947	89.805	1.00	31.37	A
45	ATOM C	1014	C	LYS A 250	245.364	-76.343	90.494	1.00	50.71	A
	ATOM O	1015	O	LYS A 250	246.506	-76.755	90.233	1.00	60.01	A
50	ATOM N	1016	N	ARG A 251	244.553	-76.931	91.389	1.00	52.78	A
	ATOM C	1017	CA	ARG A 251	244.965	-78.113	92.167	1.00	55.47	A
	ATOM C	1018	CB	ARG A 251	245.383	-79.258	91.244	1.00	58.86	A
55	ATOM C	1019	CG	ARG A 251	244.211	-79.957	90.536	1.00	62.01	A
	ATOM C	1020	CD	ARG A 251	244.126	-81.392	90.989	1.00	65.71	A
60	ATOM N	1021	NE	ARG A 251	242.807	-81.741	91.512	1.00	68.34	A
	ATOM C	1022	CZ	ARG A 251	242.484	-82.945	92.002	1.00	72.31	A

5	ATOM N	1023	NH1	ARG	A	251	243.384	-83.929	92.045	1.00	72.96	A
	ATOM N	1024	NH2	ARG	A	251	241.252	-83.178	92.445	1.00	71.74	A
	ATOM C	1025	C	ARG	A	251	246.099	-77.840	93.137	1.00	53.93	A
	ATOM O	1026	O	ARG	A	251	247.007	-78.666	93.285	1.00	57.77	A
10	ATOM N	1027	N	VAL	A	252	246.043	-76.686	93.799	1.00	56.22	A
	ATOM C	1028	CA	VAL	A	252	247.072	-76.314	94.774	1.00	53.20	A
15	ATOM C	1029	CB	VAL	A	252	247.721	-74.966	94.401	1.00	50.06	A
	ATOM C	1030	CG1	VAL	A	252	248.682	-74.549	95.463	1.00	49.54	A
	ATOM C	1031	CG2	VAL	A	252	248.418	-75.083	93.080	1.00	48.46	A
	ATOM C	1032	C	VAL	A	252	246.492	-76.207	96.196	1.00	54.67	A
20	ATOM O	1033	O	VAL	A	252	245.536	-75.465	96.426	1.00	56.55	A
	ATOM N	1034	N	ILE	A	253	247.074	-76.956	97.130	1.00	52.34	A
25	ATOM C	1035	CA	ILE	A	253	246.641	-76.948	98.498	1.00	42.71	A
	ATOM C	1036	CB	ILE	A	253	246.696	-78.341	99.103	1.00	38.24	A
30	ATOM C	1037	CG2	ILE	A	253	245.676	-78.449	100.219	1.00	44.12	A
	ATOM C	1038	CG1	ILE	A	253	246.279	-79.380	98.083	1.00	35.92	A
35	ATOM C	1039	CD1	ILE	A	253	246.298	-80.813	98.644	1.00	42.55	A
	ATOM C	1040	C	ILE	A	253	247.600	-76.096	99.279	1.00	48.08	A
	ATOM O	1041	O	ILE	A	253	248.808	-76.288	99.163	1.00	60.87	A
	ATOM N	1042	N	HIS	A	254	247.084	-75.165	100.086	1.00	50.60	A
40	ATOM C	1043	CA	HIS	A	254	247.955	-74.319	100.906	1.00	45.11	A
	ATOM C	1044	CB	HIS	A	254	247.187	-73.086	101.374	1.00	43.92	A
45	ATOM C	1045	CG	HIS	A	254	248.071	-72.014	101.916	1.00	44.85	A
	ATOM C	1046	CD2	HIS	A	254	248.486	-70.854	101.360	1.00	39.20	A
50	ATOM N	1047	ND1	HIS	A	254	248.670	-72.089	103.158	1.00	39.59	A
	ATOM C	1048	CE1	HIS	A	254	249.414	-71.014	103.339	1.00	37.61	A
55	ATOM N	1049	NE2	HIS	A	254	249.318	-70.250	102.265	1.00	38.54	A
	ATOM C	1050	C	HIS	A	254	248.490	-75.117	102.103	1.00	44.15	A
60	ATOM O	1051	O	HIS	A	254	249.681	-75.123	102.372	1.00	48.22	A
	ATOM N	1052	N	ARG	A	255	247.587	-75.802	102.793	1.00	42.94	A
	ATOM C	1053	CA	ARG	A	255	247.899	-76.642	103.946	1.00	38.93	A

Line	Atom	Res	Chain	Seq	X	Y	Z	Occup	B-factor	Alt
5	ATOM C	1054	CB	ARG A 255	248.829	-77.796	103.512	1.00	44.03	A
	ATOM C	1055	CG	ARG A 255	248.460	-78.369	102.124	1.00	46.01	A
	ATOM C	1056	CD	ARG A 255	249.154	-79.689	101.884	1.00	54.38	A
	ATOM N	1057	NE	ARG A 255	250.581	-79.648	102.175	1.00	53.55	A
10	ATOM C	1058	CZ	ARG A 255	251.402	-80.673	102.012	1.00	53.89	A
	ATOM N	1059	NH1	ARG A 255	250.938	-81.808	101.562	1.00	52.04	A
15	ATOM N	1060	NH2	ARG A 255	252.679	-80.560	102.313	1.00	55.38	A
	ATOM C	1061	C	ARG A 255	248.477	-75.929	105.145	1.00	37.93	A
20	ATOM O	1062	O	ARG A 255	248.891	-76.588	106.101	1.00	37.60	A
	ATOM N	1063	N	ASP A 256	248.541	-74.598	105.096	1.00	40.81	A
	ATOM C	1064	CA	ASP A 256	249.090	-73.852	106.231	1.00	41.86	A
	ATOM C	1065	CB	ASP A 256	250.578	-73.685	106.031	1.00	38.62	A
25	ATOM C	1066	CG	ASP A 256	251.299	-73.245	107.284	1.00	42.25	A
	ATOM O	1067	OD1	ASP A 256	250.822	-73.586	108.373	1.00	44.21	A
30	ATOM O	1068	OD2	ASP A 256	252.367	-72.594	107.177	1.00	39.16	A
	ATOM C	1069	C	ASP A 256	248.415	-72.491	106.390	1.00	45.37	A
35	ATOM O	1070	O	ASP A 256	249.065	-71.464	106.563	1.00	52.63	A
	ATOM N	1071	N	ILE A 257	247.092	-72.503	106.340	1.00	49.04	A
	ATOM C	1072	CA	ILE A 257	246.307	-71.289	106.456	1.00	56.39	A
40	ATOM C	1073	CB	ILE A 257	244.939	-71.461	105.776	1.00	52.32	A
	ATOM C	1074	CG2	ILE A 257	244.163	-70.205	105.893	1.00	55.85	A
45	ATOM C	1075	CG1	ILE A 257	245.143	-71.785	104.305	1.00	60.94	A
	ATOM C	1076	CD1	ILE A 257	243.873	-72.064	103.557	1.00	73.36	A
	ATOM C	1077	C	ILE A 257	246.097	-70.940	107.922	1.00	54.79	A
50	ATOM O	1078	O	ILE A 257	245.502	-71.720	108.659	1.00	61.06	A
	ATOM N	1079	N	LYS A 258	246.594	-69.781	108.345	1.00	50.33	A
55	ATOM C	1080	CA	LYS A 258	246.428	-69.356	109.719	1.00	46.70	A
	ATOM C	1081	CB	LYS A 258	247.273	-70.220	110.648	1.00	41.61	A
	ATOM C	1082	CG	LYS A 258	248.687	-70.371	110.232	1.00	49.22	A
60	ATOM C	1083	CD	LYS A 258	249.425	-71.326	111.200	1.00	42.38	A
	ATOM C	1084	CE	LYS A 258	250.826	-71.627	110.697	1.00	51.66	A

5	ATOM N	1085	NZ	LYS A 258	251.488	-72.718	111.456	1.00	40.89	A
	ATOM C	1086	C	LYS A 258	246.756	-67.876	109.860	1.00	45.25	A
	ATOM O	1087	O	LYS A 258	247.504	-67.337	109.042	1.00	41.75	A
	ATOM N	1088	N	PRO A 259	246.189	-67.209	110.898	1.00	38.54	A
10	ATOM C	1089	CD	PRO A 259	245.436	-67.848	111.999	1.00	30.99	A
	ATOM C	1090	CA	PRO A 259	246.389	-65.786	111.172	1.00	33.18	A
15	ATOM C	1091	CB	PRO A 259	246.034	-65.680	112.643	1.00	36.45	A
	ATOM C	1092	CG	PRO A 259	244.915	-66.649	112.762	1.00	29.46	A
20	ATOM C	1093	C	PRO A 259	247.783	-65.250	110.858	1.00	39.75	A
	ATOM O	1094	O	PRO A 259	247.899	-64.163	110.345	1.00	46.84	A
	ATOM N	1095	N	GLU A 260	248.836	-65.999	111.177	1.00	43.95	A
	ATOM C	1096	CA	GLU A 260	250.227	-65.591	110.916	1.00	44.86	A
25	ATOM C	1097	CB	GLU A 260	251.224	-66.603	111.505	1.00	50.78	A
	ATOM C	1098	CG	GLU A 260	251.039	-66.922	112.948	1.00	65.67	A
30	ATOM C	1099	CD	GLU A 260	249.918	-67.897	113.213	1.00	69.34	A
	ATOM O	1100	OE1	GLU A 260	248.727	-67.499	113.338	1.00	69.34	A
35	ATOM O	1101	OE2	GLU A 260	250.264	-69.089	113.299	1.00	80.21	A
	ATOM C	1102	C	GLU A 260	250.514	-65.476	109.430	1.00	39.11	A
	ATOM O	1103	O	GLU A 260	251.197	-64.554	109.027	1.00	44.76	A
40	ATOM N	1104	N	ASN A 261	250.029	-66.425	108.622	1.00	40.15	A
	ATOM C	1105	CA	ASN A 261	250.246	-66.396	107.162	1.00	38.92	A
	ATOM C	1106	CB	ASN A 261	250.401	-67.817	106.608	1.00	36.39	A
45	ATOM C	1107	CG	ASN A 261	251.539	-68.579	107.266	1.00	36.54	A
	ATOM O	1108	OD1	ASN A 261	252.609	-68.045	107.462	1.00	41.73	A
50	ATOM N	1109	ND2	ASN A 261	251.317	-69.831	107.578	1.00	30.81	A
	ATOM C	1110	C	ASN A 261	249.151	-65.638	106.361	1.00	38.95	A
55	ATOM O	1111	O	ASN A 261	249.142	-65.652	105.149	1.00	40.40	A
	ATOM N	1112	N	LEU A 262	248.245	-64.953	107.046	1.00	42.51	A
60	ATOM C	1113	CA	LEU A 262	247.197	-64.169	106.386	1.00	42.29	A
	ATOM C	1114	CB	LEU A 262	245.800	-64.450	106.967	1.00	36.57	A
	ATOM C	1115	CG	LEU A 262	245.209	-65.819	106.657	1.00	37.41	A

5	ATOM C	1116	CD1	LEU	A	262	243.773	-65.817	107.071	1.00	33.79	A
	ATOM C	1117	CD2	LEU	A	262	245.324	-66.152	105.193	1.00	39.29	A
10	ATOM C	1118	C	LEU	A	262	247.548	-62.703	106.582	1.00	41.70	A
	ATOM O	1119	O	LEU	A	262	247.543	-62.205	107.717	1.00	44.29	A
15	ATOM N	1120	N	LEU	A	263	247.857	-62.021	105.473	1.00	38.70	A
	ATOM C	1121	CA	LEU	A	263	248.238	-60.610	105.505	1.00	26.99	A
20	ATOM C	1122	CB	LEU	A	263	249.475	-60.392	104.679	1.00	36.05	A
	ATOM C	1123	CG	LEU	A	263	250.658	-61.333	104.917	1.00	31.41	A
25	ATOM C	1124	CD1	LEU	A	263	251.820	-60.991	103.978	1.00	33.22	A
	ATOM C	1125	CD2	LEU	A	263	251.081	-61.269	106.325	1.00	29.25	A
30	ATOM C	1126	C	LEU	A	263	247.144	-59.677	105.013	1.00	35.80	A
	ATOM O	1127	O	LEU	A	263	246.220	-60.100	104.304	1.00	32.87	A
35	ATOM N	1128	N	LEU	A	264	247.245	-58.408	105.410	1.00	31.98	A
	ATOM C	1129	CA	LEU	A	264	246.246	-57.428	105.041	1.00	33.35	A
40	ATOM C	1130	CB	LEU	A	264	245.703	-56.729	106.303	1.00	31.72	A
	ATOM C	1131	CG	LEU	A	264	244.971	-57.619	107.303	1.00	28.92	A
45	ATOM C	1132	CD1	LEU	A	264	244.728	-56.820	108.620	1.00	24.69	A
	ATOM C	1133	CD2	LEU	A	264	243.644	-58.095	106.660	1.00	26.84	A
50	ATOM C	1134	C	LEU	A	264	246.884	-56.419	104.110	1.00	35.86	A
	ATOM O	1135	O	LEU	A	264	247.974	-55.944	104.368	1.00	40.12	A
55	ATOM N	1136	N	GLY	A	265	246.188	-56.100	103.026	1.00	36.89	A
	ATOM C	1137	CA	GLY	A	265	246.674	-55.133	102.045	1.00	43.31	A
60	ATOM C	1138	C	GLY	A	265	246.399	-53.673	102.351	1.00	43.89	A
	ATOM O	1139	O	GLY	A	265	245.889	-53.350	103.401	1.00	48.54	A
65	ATOM N	1140	N	SER	A	266	246.742	-52.796	101.422	1.00	48.23	A
	ATOM C	1141	CA	SER	A	266	246.567	-51.364	101.591	1.00	49.09	A
70	ATOM C	1142	CB	SER	A	266	246.936	-50.647	100.304	1.00	51.41	A
	ATOM O	1143	OG	SER	A	266	246.057	-51.012	99.237	1.00	64.31	A
75	ATOM C	1144	C	SER	A	266	245.138	-51.019	101.970	1.00	51.39	A
	ATOM O	1145	O	SER	A	266	244.915	-50.247	102.883	1.00	54.83	A
80	ATOM N	1146	N	ALA	A	267	244.162	-51.588	101.271	1.00	54.20	A

5	ATOM C	1147	CA	ALA A 267	242.749	-51.323	101.577	1.00	47.57	A
	ATOM C	1148	CB	ALA A 267	241.921	-51.394	100.320	1.00	47.18	A
	ATOM C	1149	C	ALA A 267	242.203	-52.330	102.595	1.00	48.50	A
	ATOM O	1150	O	ALA A 267	241.010	-52.582	102.620	1.00	50.25	A
10	ATOM N	1151	N	GLY A 268	243.084	-52.913	103.410	1.00	45.91	A
	ATOM C	1152	CA	GLY A 268	242.665	-53.860	104.420	1.00	38.28	A
15	ATOM C	1153	C	GLY A 268	242.192	-55.187	103.868	1.00	42.82	A
	ATOM O	1154	O	GLY A 268	241.652	-56.003	104.639	1.00	43.08	A
	ATOM N	1155	N	GLU A 269	242.396	-55.431	102.569	1.00	42.29	A
20	ATOM C	1156	CA	GLU A 269	241.958	-56.697	101.992	1.00	40.12	A
	ATOM C	1157	CB	GLU A 269	241.996	-56.635	100.480	1.00	44.93	A
25	ATOM C	1158	CG	GLU A 269	243.430	-56.655	99.871	1.00	51.34	A
	ATOM C	1159	CD	GLU A 269	243.997	-55.261	99.657	1.00	57.16	A
	ATOM O	1160	OE1	GLU A 269	244.081	-54.491	100.642	1.00	51.07	A
30	ATOM O	1161	OE2	GLU A 269	244.350	-54.945	98.493	1.00	61.02	A
	ATOM C	1162	C	GLU A 269	242.872	-57.847	102.472	1.00	44.10	A
35	ATOM O	1163	O	GLU A 269	244.053	-57.652	102.807	1.00	43.32	A
	ATOM N	1164	N	LEU A 270	242.331	-59.059	102.481	1.00	43.44	A
	ATOM C	1165	CA	LEU A 270	243.076	-60.228	102.927	1.00	44.15	A
40	ATOM C	1166	CB	LEU A 270	242.102	-61.333	103.323	1.00	50.71	A
	ATOM C	1167	CG	LEU A 270	242.624	-62.428	104.232	1.00	53.26	A
45	ATOM C	1168	CD1	LEU A 270	242.304	-62.033	105.661	1.00	60.78	A
	ATOM C	1169	CD2	LEU A 270	241.999	-63.736	103.906	1.00	50.44	A
	ATOM C	1170	C	LEU A 270	243.985	-60.731	101.813	1.00	44.35	A
50	ATOM O	1171	O	LEU A 270	243.728	-60.526	100.635	1.00	49.43	A
	ATOM N	1172	N	LYS A 271	245.063	-61.398	102.188	1.00	40.19	A
55	ATOM C	1173	CA	LYS A 271	245.994	-61.946	101.211	1.00	31.70	A
	ATOM C	1174	CB	LYS A 271	247.028	-60.897	100.819	1.00	32.47	A
	ATOM C	1175	CG	LYS A 271	246.604	-59.930	99.753	1.00	31.86	A
60	ATOM C	1176	CD	LYS A 271	247.492	-58.692	99.731	1.00	35.87	A
	ATOM C	1177	CE	LYS A 271	247.103	-57.715	98.619	1.00	42.09	A

Atom	Res	Chain	Res	Chain	X	Y	Z	Occupancy	B-factor	Displacement
ATOM N	1178	NZ	LYS A	271	247.551	-58.225	97.303	1.00	58.37	A
ATOM C	1179	C	LYS A	271	246.714	-63.148	101.820	1.00	41.22	A
ATOM O	1180	O	LYS A	271	247.433	-63.023	102.807	1.00	49.74	A
ATOM N	1181	N	ILE A	272	246.505	-64.322	101.249	1.00	39.27	A
ATOM C	1182	CA	ILE A	272	247.155	-65.524	101.741	1.00	34.76	A
ATOM C	1183	CB	ILE A	272	246.491	-66.758	101.150	1.00	44.34	A
ATOM C	1184	CG2	ILE A	272	246.821	-67.987	102.002	1.00	55.36	A
ATOM C	1185	CG1	ILE A	272	244.973	-66.577	101.161	1.00	50.03	A
ATOM C	1186	CD1	ILE A	272	244.215	-67.794	100.577	1.00	52.97	A
ATOM C	1187	C	ILE A	272	248.617	-65.530	101.319	1.00	41.49	A
ATOM O	1188	O	ILE A	272	248.918	-65.272	100.168	1.00	40.02	A
ATOM N	1189	N	ALA A	273	249.524	-65.832	102.243	1.00	39.46	A
ATOM C	1190	CA	ALA A	273	250.936	-65.861	101.931	1.00	38.71	A
ATOM C	1191	CB	ALA A	273	251.588	-64.617	102.514	1.00	40.33	A
ATOM C	1192	C	ALA A	273	251.592	-67.137	102.487	1.00	46.92	A
ATOM O	1193	O	ALA A	273	250.910	-68.063	102.901	1.00	49.16	A
ATOM N	1194	N	ASP A	274	252.923	-67.165	102.493	1.00	51.43	A
ATOM C	1195	CA	ASP A	274	253.703	-68.293	102.997	1.00	51.40	A
ATOM C	1196	CB	ASP A	274	253.686	-68.323	104.530	1.00	50.98	A
ATOM C	1197	CG	ASP A	274	254.601	-69.361	105.083	1.00	42.10	A
ATOM O	1198	OD1	ASP A	274	255.660	-69.637	104.516	1.00	54.26	A
ATOM O	1199	OD2	ASP A	274	254.299	-69.914	106.121	1.00	52.11	A
ATOM C	1200	C	ASP A	274	253.224	-69.618	102.433	1.00	51.38	A
ATOM O	1201	O	ASP A	274	252.572	-70.382	103.133	1.00	53.85	A
ATOM N	1202	N	PHE A	275	253.540	-69.863	101.159	1.00	53.60	A
ATOM C	1203	CA	PHE A	275	253.173	-71.097	100.476	1.00	46.97	A
ATOM C	1204	CB	PHE A	275	252.975	-70.871	98.973	1.00	42.90	A
ATOM C	1205	CG	PHE A	275	251.733	-70.169	98.636	1.00	45.54	A
ATOM C	1206	CD1	PHE A	275	251.527	-68.830	99.048	1.00	45.75	A
ATOM C	1207	CD2	PHE A	275	250.737	-70.843	97.917	1.00	41.77	A
ATOM C	1208	CE1	PHE A	275	250.305	-68.152	98.737	1.00	48.01	A

5	ATOM C	1209	CE2	PHE A 275	249.503	-70.195	97.591	1.00	46.76	A
	ATOM C	1210	CZ	PHE A 275	249.279	-68.840	98.000	1.00	48.77	A
	ATOM C	1211	C	PHE A 275	254.270	-72.149	100.678	1.00	43.41	A
	ATOM O	1212	O	PHE A 275	254.496	-72.970	99.791	1.00	36.81	A
10	ATOM N	1213	N	GLY A 276	254.938	-72.109	101.843	1.00	42.93	A
	ATOM C	1214	CA	GLY A 276	255.969	-73.079	102.214	1.00	37.83	A
15	ATOM C	1215	C	GLY A 276	255.471	-74.522	102.210	1.00	35.71	A
	ATOM O	1216	O	GLY A 276	256.197	-75.412	101.834	1.00	45.98	A
20	ATOM N	1217	N	TRP A 277	254.227	-74.768	102.608	1.00	40.57	A
	ATOM C	1218	CA	TRP A 277	253.676	-76.118	102.591	1.00	36.62	A
	ATOM C	1219	CB	TRP A 277	252.882	-76.378	103.859	1.00	42.09	A
	ATOM C	1220	CG	TRP A 277	253.751	-76.592	105.041	1.00	50.97	A
25	ATOM C	1221	CD2	TRP A 277	254.089	-77.854	105.629	1.00	58.62	A
	ATOM C	1222	CE2	TRP A 277	254.960	-77.593	106.702	1.00	58.91	A
30	ATOM C	1223	CE3	TRP A 277	253.726	-79.182	105.360	1.00	59.93	A
	ATOM C	1224	CD1	TRP A 277	254.420	-75.640	105.759	1.00	54.30	A
35	ATOM N	1225	NE1	TRP A 277	255.150	-76.235	106.758	1.00	59.86	A
	ATOM C	1226	CZ2	TRP A 277	255.482	-78.610	107.501	1.00	61.19	A
	ATOM C	1227	CZ3	TRP A 277	254.244	-80.188	106.162	1.00	61.29	A
40	ATOM C	1228	CH2	TRP A 277	255.108	-79.892	107.219	1.00	63.73	A
	ATOM C	1229	C	TRP A 277	252.777	-76.364	101.408	1.00	35.74	A
45	ATOM O	1230	O	TRP A 277	252.212	-77.442	101.298	1.00	35.61	A
	ATOM N	1231	N	SER A 278	252.636	-75.372	100.528	1.00	44.94	A
50	ATOM C	1232	CA	SER A 278	251.779	-75.474	99.336	1.00	46.77	A
	ATOM C	1233	CB	SER A 278	251.916	-74.202	98.517	1.00	42.80	A
	ATOM O	1234	OG	SER A 278	250.880	-74.139	97.565	1.00	54.88	A
55	ATOM C	1235	C	SER A 278	252.200	-76.703	98.464	1.00	50.47	A
	ATOM O	1236	O	SER A 278	253.367	-77.084	98.378	1.00	54.17	A
60	ATOM N	1237	N	VAL A 279	251.246	-77.347	97.819	1.00	51.50	A
	ATOM C	1238	CA	VAL A 279	251.566	-78.514	96.992	1.00	57.94	A
	ATOM C	1239	CB	VAL A 279	251.588	-79.780	97.847	1.00	44.98	A

5	ATOM C	1240	CG1	VAL	A	279	250.199	-80.321	97.997	1.00	43.31	A
	ATOM C	1241	CG2	VAL	A	279	252.491	-80.787	97.178	1.00	57.04	A
	ATOM C	1242	C	VAL	A	279	250.626	-78.680	95.765	1.00	59.15	A
	ATOM O	1243	O	VAL	A	279	249.430	-78.387	95.867	1.00	67.05	A
10	ATOM N	1244	N	HIS	A	280	251.204	-79.094	94.615	1.00	63.81	A
	ATOM C	1245	CA	HIS	A	280	250.486	-79.252	93.335	1.00	67.43	A
15	ATOM C	1246	CB	HIS	A	280	251.439	-79.066	92.122	1.00	66.79	A
	ATOM C	1247	CG	HIS	A	280	250.875	-78.185	91.056	1.00	72.05	A
20	ATOM C	1248	CD2	HIS	A	280	250.729	-78.371	89.721	1.00	75.11	A
	ATOM N	1249	ND1	HIS	A	280	250.404	-76.921	91.326	1.00	73.34	A
	ATOM C	1250	CE1	HIS	A	280	249.997	-76.358	90.201	1.00	80.03	A
25	ATOM N	1251	NE2	HIS	A	280	250.185	-77.217	89.213	1.00	83.14	A
	ATOM C	1252	C	HIS	A	280	249.968	-80.672	93.390	1.00	70.50	A
30	ATOM O	1253	O	HIS	A	280	250.581	-81.589	92.745	1.00	82.51	A
	ATOM N	1254	N	ALA	A	281	248.772	-80.853	93.985	1.00	68.02	A
	ATOM C	1255	CA	ALA	A	281	248.427	-82.260	94.196	1.00	68.33	A
35	ATOM C	1256	CB	ALA	A	281	249.603	-82.885	94.806	1.00	60.98	A
	ATOM C	1257	C	ALA	A	281	247.205	-82.754	95.016	1.00	68.64	A
40	ATOM O	1258	O	ALA	A	281	246.292	-82.032	95.339	1.00	67.99	A
	ATOM N	1259	N	PRO	A	282	247.225	-84.034	95.373	1.00	70.43	A
	ATOM C	1260	CD	PRO	A	282	246.861	-84.236	93.943	1.00	64.78	A
45	ATOM C	1261	CA	PRO	A	282	246.609	-85.171	96.058	1.00	67.06	A
	ATOM C	1262	CB	PRO	A	282	246.654	-86.295	95.053	1.00	67.65	A
50	ATOM C	1263	CG	PRO	A	282	246.201	-85.826	93.934	1.00	63.34	A
	ATOM C	1264	C	PRO	A	282	247.893	-85.384	96.902	1.00	69.62	A
	ATOM O	1265	O	PRO	A	282	248.995	-85.628	96.346	1.00	80.00	A
55	ATOM N	1266	N	SER	A	283	247.878	-85.322	98.204	1.00	65.02	A
	ATOM C	1267	CA	SER	A	283	249.163	-85.680	98.758	1.00	59.53	A
60	ATOM C	1268	CB	SER	A	283	250.127	-84.498	98.799	1.00	55.46	A
	ATOM O	1269	OG	SER	A	283	250.750	-84.456	100.075	1.00	55.84	A
	ATOM C	1270	C	SER	A	283	249.259	-86.394	100.033	1.00	55.99	A

Atom	ID	Type	Res	Chain	X (Å)	Y (Å)	Z (Å)	Occupancy	B-factor (Å ²)	Disorder
ATOM O	1271	O	SER	A 283	248.283	-86.609	100.713	1.00	69.93	A
ATOM N	1272	N	SER	A 284	250.462	-86.835	100.323	1.00	60.56	A
ATOM C	1273	CA	SER	A 284	250.699	-87.467	101.588	1.00	63.49	A
ATOM C	1274	CB	SER	A 284	251.416	-88.808	101.438	1.00	63.76	A
ATOM O	1275	OG	SER	A 284	252.588	-88.697	100.633	1.00	77.24	A
ATOM C	1276	C	SER	A 284	251.609	-86.432	102.280	1.00	63.54	A
ATOM O	1277	O	SER	A 284	251.934	-85.336	101.744	1.00	57.98	A
ATOM N	1278	N	ARG	A 285	251.999	-86.775	103.492	1.00	64.16	A
ATOM C	1279	CA	ARG	A 285	252.823	-85.889	104.282	1.00	67.66	A
ATOM C	1280	CB	ARG	A 285	252.738	-86.301	105.734	1.00	62.91	A
ATOM C	1281	C	ARG	A 285	254.278	-85.923	103.806	1.00	68.61	A
ATOM O	1282	O	ARG	A 285	254.612	-86.645	102.888	1.00	72.84	A
ATOM N	1283	N	ARG	A 286	255.135	-85.146	104.466	1.00	71.24	A
ATOM C	1284	CA	ARG	A 286	256.561	-85.059	104.163	1.00	75.06	A
ATOM C	1285	CB	ARG	A 286	256.943	-83.563	104.008	1.00	73.44	A
ATOM C	1286	CG	ARG	A 286	255.881	-82.698	103.382	1.00	71.75	A
ATOM C	1287	CD	ARG	A 286	255.139	-83.449	102.361	1.00	72.37	A
ATOM N	1288	NE	ARG	A 286	255.481	-82.999	101.030	1.00	72.92	A
ATOM C	1289	CZ	ARG	A 286	254.690	-83.207	99.989	1.00	77.01	A
ATOM N	1290	NH1	ARG	A 286	253.537	-83.858	100.174	1.00	80.80	A
ATOM N	1291	NH2	ARG	A 286	255.024	-82.753	98.778	1.00	73.00	A
ATOM C	1292	C	ARG	A 286	257.251	-85.649	105.339	1.00	79.18	A
ATOM O	1293	O	ARG	A 286	258.525	-85.258	105.556	1.00	80.60	A
ATOM N	1294	N	TPO	A 287	256.458	-86.471	106.097	1.00	82.59	A
ATOM C	1295	CA	TPO	A 287	256.848	-87.091	107.376	1.00	81.36	A
ATOM C	1296	CB	TPO	A 287	258.340	-87.583	107.506	1.00	85.77	A
ATOM C	1297	CG2	TPO	A 287	258.788	-88.436	108.791	1.00	78.62	A
ATOM O	1298	OG1	TPO	A 287	259.242	-87.965	106.406	1.00	96.25	A
ATOM P	1299	P	TPO	A 287	259.671	-89.537	105.840	1.00	94.10	A
ATOM O	1300	O1P	TPO	A 287	261.195	-89.889	106.372	1.00	105.80	A
ATOM O	1301	O2P	TPO	A 287	259.793	-89.485	104.142	1.00	103.14	A

	ATOM	1302	O3P	TPO A 287	258.773	-90.552	106.786	1.00103.19	A
	O								
	ATOM	1303	C	TPO A 287	257.020	-86.093	108.560	1.00 84.40	A
	C								
5	ATOM	1304	O	TPO A 287	256.708	-86.453	109.760	1.00 82.15	A
	O								
	ATOM	1305	N	TPO A 288	257.164	-84.776	108.357	1.00 86.52	A
	N								
10	ATOM	1306	CA	TPO A 288	257.256	-84.113	109.592	1.00 85.55	A
	C								
	ATOM	1307	CB	TPO A 288	258.562	-83.387	109.678	1.00 87.59	A
	C								
	ATOM	1308	CG2	TPO A 288	259.265	-83.063	111.066	1.00 82.26	A
	C								
15	ATOM	1309	OG1	TPO A 288	259.687	-83.759	108.739	1.00 93.55	A
	O								
	ATOM	1310	P	TPO A 288	261.048	-84.822	108.978	1.00 87.77	A
	P								
20	ATOM	1311	O1P	TPO A 288	262.388	-83.892	109.216	1.00 91.79	A
	O								
	ATOM	1312	O2P	TPO A 288	261.352	-85.656	107.542	1.00 93.35	A
	O								
	ATOM	1313	O3P	TPO A 288	260.797	-85.456	110.481	1.00 95.16	A
	O								
25	ATOM	1314	C	TPO A 288	256.287	-82.985	109.892	1.00 89.28	A
	C								
	ATOM	1315	O	TPO A 288	255.311	-82.594	109.048	1.00 86.14	A
	O								
30	ATOM	1316	N	LEU A 289	256.536	-82.411	111.055	1.00 87.01	A
	N								
	ATOM	1317	CA	LEU A 289	255.511	-81.523	111.435	1.00 88.25	A
	C								
	ATOM	1318	CB	LEU A 289	254.346	-82.345	111.883	1.00 78.91	A
	C								
35	ATOM	1319	C	LEU A 289	255.852	-80.565	112.436	1.00 87.34	A
	C								
	ATOM	1320	O	LEU A 289	256.026	-80.894	113.634	1.00 90.27	A
	O								
40	ATOM	1321	N	CYS A 290	256.101	-79.389	111.914	1.00 89.51	A
	N								
	ATOM	1322	CA	CYS A 290	256.347	-78.354	112.824	1.00 89.73	A
	C								
	ATOM	1323	CB	CYS A 290	257.299	-77.405	112.324	1.00 80.05	A
	C								
45	ATOM	1324	C	CYS A 290	254.931	-77.891	112.490	1.00 90.22	A
	C								
	ATOM	1325	O	CYS A 290	254.405	-77.933	111.292	1.00 91.11	A
	O								
50	ATOM	1326	N	GLY A 291	254.262	-77.496	113.541	1.00 90.88	A
	N								
	ATOM	1327	CA	GLY A 291	252.946	-77.026	113.294	1.00 84.36	A
	C								
	ATOM	1328	C	GLY A 291	252.214	-77.175	114.559	1.00 80.67	A
	C								
55	ATOM	1329	O	GLY A 291	252.395	-78.093	115.381	1.00 72.19	A
	O								
	ATOM	1330	N	THR A 292	251.411	-76.152	114.668	1.00 72.87	A
	N								
60	ATOM	1331	CA	THR A 292	250.543	-75.923	115.732	1.00 68.66	A
	C								
	ATOM	1332	CB	THR A 292	250.229	-74.450	115.788	1.00 64.26	A
	C								

5	ATOM O	1333	OG1	THR	A	292	249.385	-74.238	116.907	1.00	62.83	A
	ATOM C	1334	CG2	THR	A	292	249.511	-73.967	114.478	1.00	66.76	A
	ATOM C	1335	C	THR	A	292	249.401	-76.698	115.093	1.00	69.67	A
	ATOM O	1336	O	THR	A	292	248.736	-76.230	114.162	1.00	81.32	A
10	ATOM N	1337	N	LEU	A	293	249.162	-77.905	115.545	1.00	65.76	A
	ATOM C	1338	CA	LEU	A	293	248.076	-78.633	114.929	1.00	57.85	A
15	ATOM C	1339	CB	LEU	A	293	247.775	-79.863	115.741	1.00	58.26	A
	ATOM C	1340	CG	LEU	A	293	249.007	-80.649	116.175	1.00	59.75	A
20	ATOM C	1341	CD1	LEU	A	293	248.607	-81.606	117.246	1.00	56.85	A
	ATOM C	1342	CD2	LEU	A	293	249.618	-81.397	114.982	1.00	55.33	A
	ATOM C	1343	C	LEU	A	293	246.812	-77.819	114.737	1.00	54.37	A
25	ATOM O	1344	O	LEU	A	293	246.215	-77.930	113.686	1.00	59.11	A
	ATOM N	1345	N	ASP	A	294	246.467	-76.947	115.687	1.00	45.72	A
	ATOM C	1346	CA	ASP	A	294	245.241	-76.166	115.622	1.00	46.04	A
30	ATOM C	1347	CB	ASP	A	294	245.471	-74.762	116.195	1.00	47.18	A
	ATOM C	1348	CG	ASP	A	294	245.754	-74.782	117.713	1.00	53.87	A
35	ATOM O	1349	OD1	ASP	A	294	244.938	-75.399	118.452	1.00	53.07	A
	ATOM O	1350	OD2	ASP	A	294	246.772	-74.166	118.153	1.00	44.18	A
	ATOM C	1351	C	ASP	A	294	244.490	-76.064	114.323	1.00	42.63	A
40	ATOM O	1352	O	ASP	A	294	243.322	-76.434	114.275	1.00	40.46	A
	ATOM N	1353	N	TYR	A	295	245.168	-75.589	113.280	1.00	41.51	A
45	ATOM C	1354	CA	TYR	A	295	244.534	-75.404	111.983	1.00	42.29	A
	ATOM C	1355	CB	TYR	A	295	245.046	-74.116	111.335	1.00	42.13	A
50	ATOM C	1356	CG	TYR	A	295	245.120	-72.945	112.263	1.00	41.89	A
	ATOM C	1357	CD1	TYR	A	295	246.211	-72.793	113.099	1.00	47.14	A
	ATOM C	1358	CE1	TYR	A	295	246.304	-71.731	113.973	1.00	47.33	A
55	ATOM C	1359	CD2	TYR	A	295	244.117	-71.995	112.309	1.00	36.13	A
	ATOM C	1360	CE2	TYR	A	295	244.212	-70.914	113.162	1.00	43.23	A
60	ATOM C	1361	CZ	TYR	A	295	245.302	-70.785	113.996	1.00	47.19	A
	ATOM O	1362	OH	TYR	A	295	245.414	-69.690	114.838	1.00	57.32	A
	ATOM C	1363	C	TYR	A	295	244.655	-76.563	110.985	1.00	41.49	A

Residue	Atom	Res	Chain	Seq	X	Y	Z	Occup	B-factor	Alt
5	ATOM O	1364	O	TYR A 295	244.224	-76.467	109.822	1.00	43.26	A
	ATOM N	1365	N	LEU A 296	245.228	-77.668	111.448	1.00	39.99	A
	ATOM C	1366	CA	LEU A 296	245.411	-78.868	110.607	1.00	51.39	A
	ATOM C	1367	CB	LEU A 296	246.671	-79.611	111.016	1.00	53.81	A
10	ATOM C	1368	CG	LEU A 296	248.033	-78.987	110.652	1.00	57.41	A
	ATOM C	1369	CD1	LEU A 296	249.165	-79.934	111.025	1.00	51.84	A
15	ATOM C	1370	CD2	LEU A 296	248.040	-78.694	109.161	1.00	50.59	A
	ATOM C	1371	C	LEU A 296	244.205	-79.803	110.651	1.00	48.90	A
20	ATOM O	1372	O	LEU A 296	243.511	-79.890	111.645	1.00	60.00	A
	ATOM N	1373	N	PRO A 297	243.914	-80.480	109.550	1.00	49.64	A
	ATOM C	1374	CD	PRO A 297	244.428	-80.152	108.220	1.00	48.93	A
	ATOM C	1375	CA	PRO A 297	242.782	-81.390	109.447	1.00	53.31	A
25	ATOM C	1376	CB	PRO A 297	242.450	-81.327	107.951	1.00	50.04	A
	ATOM C	1377	CG	PRO A 297	243.782	-81.194	107.367	1.00	48.93	A
30	ATOM C	1378	C	PRO A 297	243.137	-82.762	109.966	1.00	57.23	A
	ATOM O	1379	O	PRO A 297	244.303	-83.109	110.051	1.00	56.18	A
35	ATOM N	1380	N	PRO A 298	242.135	-83.562	110.334	1.00	59.72	A
	ATOM C	1381	CD	PRO A 298	240.704	-83.237	110.308	1.00	64.33	A
	ATOM C	1382	CA	PRO A 298	242.340	-84.917	110.853	1.00	62.61	A
40	ATOM C	1383	CB	PRO A 298	240.929	-85.463	110.920	1.00	65.22	A
	ATOM C	1384	CG	PRO A 298	240.143	-84.267	111.288	1.00	64.88	A
45	ATOM C	1385	C	PRO A 298	243.245	-85.779	109.963	1.00	64.63	A
	ATOM O	1386	O	PRO A 298	244.184	-86.426	110.459	1.00	56.23	A
	ATOM N	1387	N	GLU A 299	242.975	-85.781	108.656	1.00	60.03	A
50	ATOM C	1388	CA	GLU A 299	243.778	-86.574	107.711	1.00	58.56	A
	ATOM C	1389	CB	GLU A 299	243.303	-86.339	106.265	1.00	57.01	A
55	ATOM C	1390	CG	GLU A 299	243.028	-84.864	105.914	1.00	52.94	A
	ATOM C	1391	CD	GLU A 299	241.596	-84.474	106.109	1.00	48.80	A
60	ATOM O	1392	OE1	GLU A 299	241.003	-84.897	107.126	1.00	47.74	A
	ATOM O	1393	OE2	GLU A 299	241.075	-83.733	105.248	1.00	48.97	A
	ATOM C	1394	C	GLU A 299	245.279	-86.287	107.819	1.00	62.41	A

5	ATOM O	1395	O	GLU A 299	246.094	-87.208	108.002	1.00	64.05	A
	ATOM N	1396	N	MET A 300	245.648	-85.014	107.709	1.00	63.79	A
	ATOM C	1397	CA	MET A 300	247.051	-84.637	107.816	1.00	63.71	A
	ATOM C	1398	CB	MET A 300	247.225	-83.145	107.597	1.00	67.63	A
10	ATOM C	1399	CG	MET A 300	247.374	-82.763	106.145	1.00	66.70	A
	ATOM S	1400	SD	MET A 300	248.052	-81.127	106.017	1.00	71.20	A
15	ATOM C	1401	CE	MET A 300	249.750	-81.388	106.380	1.00	69.10	A
	ATOM C	1402	C	MET A 300	247.661	-85.000	109.174	1.00	66.02	A
20	ATOM O	1403	O	MET A 300	248.702	-85.664	109.256	1.00	70.05	A
	ATOM N	1404	N	ILE A 301	247.025	-84.550	110.244	1.00	67.53	A
	ATOM C	1405	CA	ILE A 301	247.504	-84.829	111.596	1.00	68.63	A
	ATOM C	1406	CB	ILE A 301	246.490	-84.278	112.606	1.00	67.77	A
25	ATOM C	1407	CG2	ILE A 301	246.782	-84.750	113.995	1.00	61.97	A
	ATOM C	1408	CG1	ILE A 301	246.505	-82.750	112.495	1.00	67.98	A
30	ATOM C	1409	CD1	ILE A 301	245.392	-82.041	113.240	1.00	76.63	A
	ATOM C	1410	C	ILE A 301	247.769	-86.319	111.812	1.00	73.57	A
35	ATOM O	1411	O	ILE A 301	248.662	-86.676	112.588	1.00	78.37	A
	ATOM N	1412	N	GLU A 302	247.034	-87.184	111.092	1.00	75.18	A
	ATOM C	1413	CA	GLU A 302	247.212	-88.639	111.215	1.00	74.73	A
40	ATOM C	1414	CB	GLU A 302	245.845	-89.306	111.428	1.00	70.49	A
	ATOM C	1415	CG	GLU A 302	245.378	-89.254	112.936	1.00	78.38	A
45	ATOM C	1416	CD	GLU A 302	243.861	-89.396	113.127	1.00	79.55	A
	ATOM O	1417	OE1	GLU A 302	243.188	-90.062	112.281	1.00	80.35	A
	ATOM O	1418	OE2	GLU A 302	243.360	-88.836	114.140	1.00	87.62	A
50	ATOM C	1419	C	GLU A 302	248.026	-89.290	110.065	1.00	75.98	A
	ATOM O	1420	O	GLU A 302	248.411	-90.458	110.160	1.00	81.76	A
55	ATOM N	1421	N	GLY A 303	248.339	-88.531	109.006	1.00	78.40	A
	ATOM C	1422	CA	GLY A 303	249.160	-89.053	107.912	1.00	72.91	A
	ATOM C	1423	C	GLY A 303	248.566	-89.374	106.552	1.00	72.79	A
60	ATOM O	1424	O	GLY A 303	249.237	-89.368	105.513	1.00	76.85	A
	ATOM N	1425	N	ARG A 304	247.286	-89.679	106.549	1.00	67.34	A

Row	Atom	ID	Res	Type	Chain	Seq	X	Y	Z	Occ	B	Alt
5	ATOM C	1426	CA	ARG	A	304	246.623	-90.043	105.300	1.00	63.57	A
	ATOM C	1427	CB	ARG	A	304	245.098	-90.120	105.461	1.00	62.11	A
	ATOM C	1428	CG	ARG	A	304	244.623	-91.200	106.414	1.00	63.49	A
	ATOM C	1429	CD	ARG	A	304	243.198	-90.950	106.857	1.00	70.18	A
10	ATOM N	1430	NE	ARG	A	304	243.087	-89.787	107.759	1.00	79.24	A
	ATOM C	1431	CZ	ARG	A	304	242.896	-89.857	109.080	1.00	78.33	A
15	ATOM N	1432	NH1	ARG	A	304	242.788	-91.031	109.665	1.00	78.68	A
	ATOM N	1433	NH2	ARG	A	304	242.819	-88.757	109.821	1.00	83.87	A
	ATOM C	1434	C	ARG	A	304	246.882	-89.200	104.087	1.00	60.49	A
20	ATOM O	1435	O	ARG	A	304	247.550	-88.195	104.122	1.00	65.51	A
	ATOM N	1436	N	MET	A	305	246.278	-89.661	103.013	1.00	61.50	A
25	ATOM C	1437	CA	MET	A	305	246.335	-89.084	101.698	1.00	65.46	A
	ATOM C	1438	CB	MET	A	305	246.041	-90.197	100.663	1.00	63.39	A
	ATOM C	1439	C	MET	A	305	245.233	-88.042	101.699	1.00	69.37	A
30	ATOM O	1440	O	MET	A	305	244.036	-88.349	101.691	1.00	78.96	A
	ATOM N	1441	N	HIS	A	306	245.671	-86.802	101.710	1.00	69.56	A
35	ATOM C	1442	CA	HIS	A	306	244.790	-85.674	101.706	1.00	64.25	A
	ATOM C	1443	CB	HIS	A	306	245.247	-84.657	102.735	1.00	64.47	A
	ATOM C	1444	CG	HIS	A	306	246.674	-84.276	102.611	1.00	58.72	A
40	ATOM C	1445	CD2	HIS	A	306	247.253	-83.167	102.099	1.00	56.35	A
	ATOM N	1446	ND1	HIS	A	306	247.691	-85.072	103.092	1.00	58.38	A
45	ATOM C	1447	CE1	HIS	A	306	248.841	-84.461	102.883	1.00	55.77	A
	ATOM N	1448	NE2	HIS	A	306	248.602	-83.307	102.284	1.00	54.24	A
	ATOM C	1449	C	HIS	A	306	244.657	-85.001	100.363	1.00	64.13	A
50	ATOM O	1450	O	HIS	A	306	245.469	-85.186	99.467	1.00	61.51	A
	ATOM N	1451	N	ASP	A	307	243.667	-84.122	100.305	1.00	66.29	A
55	ATOM C	1452	CA	ASP	A	307	243.316	-83.353	99.117	1.00	67.53	A
	ATOM C	1453	CB	ASP	A	307	241.988	-83.886	98.618	1.00	76.36	A
	ATOM C	1454	CG	ASP	A	307	241.022	-84.130	99.789	1.00	82.91	A
60	ATOM O	1455	OD1	ASP	A	307	240.938	-83.232	100.665	1.00	87.78	A
	ATOM O	1456	OD2	ASP	A	307	240.376	-85.208	99.863	1.00	84.54	A

5	ATOM C	1457	C	ASP A 307	243.130	-81.873	99.495	1.00	62.06	A
	ATOM O	1458	O	ASP A 307	243.430	-81.435	100.603	1.00	62.07	A
	ATOM N	1459	N	GLU A 308	242.537	-81.150	98.566	1.00	56.29	A
	ATOM C	1460	CA	GLU A 308	242.256	-79.740	98.709	1.00	59.89	A
	ATOM C	1461	CB	GLU A 308	241.830	-79.236	97.325	1.00	58.22	A
10	ATOM C	1462	CG	GLU A 308	241.947	-80.428	96.353	1.00	63.76	A
	ATOM C	1463	CD	GLU A 308	241.729	-80.087	94.898	1.00	66.66	A
	ATOM O	1464	OE1	GLU A 308	242.570	-79.367	94.305	1.00	69.11	A
15	ATOM O	1465	OE2	GLU A 308	240.722	-80.565	94.330	1.00	69.49	A
	ATOM C	1466	C	GLU A 308	241.201	-79.444	99.802	1.00	56.96	A
	ATOM O	1467	O	GLU A 308	241.003	-78.286	100.226	1.00	57.79	A
20	ATOM N	1468	N	LYS A 309	240.558	-80.495	100.296	1.00	54.61	A
	ATOM C	1469	CA	LYS A 309	239.526	-80.332	101.317	1.00	54.70	A
	ATOM C	1470	CB	LYS A 309	238.697	-81.615	101.449	1.00	46.40	A
25	ATOM C	1471	CG	LYS A 309	237.740	-81.859	100.300	1.00	53.44	A
	ATOM C	1472	CD	LYS A 309	236.674	-80.778	100.253	1.00	58.61	A
	ATOM C	1473	CE	LYS A 309	235.600	-81.071	99.214	1.00	60.43	A
30	ATOM N	1474	NZ	LYS A 309	234.524	-80.026	99.209	1.00	60.76	A
	ATOM C	1475	C	LYS A 309	240.111	-79.967	102.668	1.00	54.64	A
	ATOM O	1476	O	LYS A 309	239.366	-79.724	103.618	1.00	66.35	A
35	ATOM N	1477	N	VAL A 310	241.439	-79.941	102.770	1.00	57.91	A
	ATOM C	1478	CA	VAL A 310	242.086	-79.593	104.039	1.00	53.66	A
	ATOM C	1479	CB	VAL A 310	243.573	-79.974	104.058	1.00	52.18	A
40	ATOM C	1480	CG1	VAL A 310	243.749	-81.375	103.528	1.00	54.98	A
	ATOM C	1481	CG2	VAL A 310	244.347	-79.010	103.252	1.00	55.72	A
	ATOM C	1482	C	VAL A 310	241.957	-78.091	104.263	1.00	53.64	A
45	ATOM O	1483	O	VAL A 310	241.771	-77.638	105.404	1.00	47.54	A
	ATOM N	1484	N	ASP A 311	242.008	-77.332	103.168	1.00	50.01	A
	ATOM C	1485	CA	ASP A 311	241.881	-75.889	103.255	1.00	57.45	A
50	ATOM C	1486	CB	ASP A 311	242.275	-75.232	101.925	1.00	56.10	A
	ATOM C	1487	CG	ASP A 311	243.756	-75.367	101.624	1.00	55.84	A

5	ATOM O	1488	OD1	ASP	A	311	244.585	-75.238	102.553	1.00	49.03	A
	ATOM O	1489	OD2	ASP	A	311	244.085	-75.597	100.453	1.00	54.46	A
	ATOM C	1490	C	ASP	A	311	240.454	-75.467	103.667	1.00	59.07	A
	ATOM O	1491	O	ASP	A	311	240.258	-74.365	104.208	1.00	69.75	A
10	ATOM N	1492	N	LEU	A	312	239.471	-76.343	103.445	1.00	56.37	A
	ATOM C	1493	CA	LEU	A	312	238.117	-76.031	103.815	1.00	45.08	A
15	ATOM C	1494	CB	LEU	A	312	237.135	-76.975	103.126	1.00	46.93	A
	ATOM C	1495	CG	LEU	A	312	236.719	-76.481	101.746	1.00	45.65	A
	ATOM C	1496	CD1	LEU	A	312	236.262	-77.698	100.966	1.00	57.08	A
20	ATOM C	1497	CD2	LEU	A	312	235.607	-75.431	101.878	1.00	42.14	A
	ATOM C	1498	C	LEU	A	312	238.066	-76.204	105.309	1.00	42.72	A
25	ATOM O	1499	O	LEU	A	312	237.357	-75.451	105.986	1.00	41.50	A
	ATOM N	1500	N	TRP	A	313	238.778	-77.211	105.814	1.00	35.13	A
	ATOM C	1501	CA	TRP	A	313	238.818	-77.454	107.257	1.00	42.05	A
30	ATOM C	1502	CB	TRP	A	313	239.630	-78.718	107.532	1.00	37.59	A
	ATOM C	1503	CG	TRP	A	313	239.903	-78.960	108.973	1.00	37.21	A
35	ATOM C	1504	CD2	TRP	A	313	239.169	-79.815	109.859	1.00	38.09	A
	ATOM C	1505	CE2	TRP	A	313	239.786	-79.742	111.133	1.00	40.55	A
	ATOM C	1506	CE3	TRP	A	313	238.050	-80.627	109.706	1.00	42.38	A
40	ATOM C	1507	CD1	TRP	A	313	240.895	-78.418	109.716	1.00	40.67	A
	ATOM N	1508	NE1	TRP	A	313	240.843	-78.885	111.022	1.00	36.83	A
45	ATOM C	1509	CZ2	TRP	A	313	239.325	-80.470	112.237	1.00	41.12	A
	ATOM C	1510	CZ3	TRP	A	313	237.591	-81.353	110.817	1.00	40.98	A
	ATOM C	1511	CH2	TRP	A	313	238.220	-81.265	112.052	1.00	42.79	A
50	ATOM C	1512	C	TRP	A	313	239.448	-76.259	108.009	1.00	45.03	A
	ATOM O	1513	O	TRP	A	313	238.971	-75.813	109.044	1.00	49.94	A
55	ATOM N	1514	N	SER	A	314	240.543	-75.748	107.477	1.00	46.02	A
	ATOM C	1515	CA	SER	A	314	241.220	-74.624	108.087	1.00	41.93	A
	ATOM C	1516	CB	SER	A	314	242.523	-74.354	107.341	1.00	44.32	A
60	ATOM O	1517	OG	SER	A	314	243.333	-75.505	107.387	1.00	38.93	A
	ATOM C	1518	C	SER	A	314	240.338	-73.392	108.062	1.00	39.99	A

5	ATOM O	1519	O	SER A 314	240.328	-72.596	109.011	1.00	45.37	A
	ATOM N	1520	N	LEU A 315	239.616	-73.226	106.965	1.00	35.87	A
	ATOM C	1521	CA	LEU A 315	238.704	-72.091	106.805	1.00	35.10	A
	ATOM C	1522	CB	LEU A 315	238.115	-72.091	105.390	1.00	34.40	A
10	ATOM C	1523	CG	LEU A 315	237.307	-70.872	104.991	1.00	41.64	A
	ATOM C	1524	CD1	LEU A 315	238.136	-69.564	105.204	1.00	42.79	A
15	ATOM C	1525	CD2	LEU A 315	236.927	-71.022	103.523	1.00	40.03	A
	ATOM C	1526	C	LEU A 315	237.569	-72.154	107.851	1.00	38.86	A
20	ATOM O	1527	O	LEU A 315	236.854	-71.200	108.035	1.00	42.90	A
	ATOM N	1528	N	GLY A 316	237.421	-73.301	108.515	1.00	40.90	A
	ATOM C	1529	CA	GLY A 316	236.420	-73.475	109.540	1.00	29.38	A
25	ATOM C	1530	C	GLY A 316	237.051	-73.072	110.863	1.00	38.31	A
	ATOM O	1531	O	GLY A 316	236.444	-72.317	111.644	1.00	44.99	A
30	ATOM N	1532	N	VAL A 317	238.259	-73.578	111.126	1.00	34.77	A
	ATOM C	1533	CA	VAL A 317	238.980	-73.253	112.343	1.00	38.52	A
	ATOM C	1534	CB	VAL A 317	240.378	-73.903	112.348	1.00	39.35	A
35	ATOM C	1535	CG1	VAL A 317	241.200	-73.322	113.465	1.00	39.07	A
	ATOM C	1536	CG2	VAL A 317	240.268	-75.403	112.500	1.00	36.59	A
40	ATOM C	1537	C	VAL A 317	239.145	-71.743	112.382	1.00	39.43	A
	ATOM O	1538	O	VAL A 317	238.923	-71.092	113.421	1.00	39.97	A
	ATOM N	1539	N	LEU A 318	239.517	-71.195	111.226	1.00	35.94	A
45	ATOM C	1540	CA	LEU A 318	239.728	-69.769	111.107	1.00	35.49	A
	ATOM C	1541	CB	LEU A 318	240.217	-69.443	109.701	1.00	34.72	A
50	ATOM C	1542	CG	LEU A 318	241.505	-68.678	109.594	1.00	35.85	A
	ATOM C	1543	CD1	LEU A 318	242.492	-69.129	110.631	1.00	35.87	A
	ATOM C	1544	CD2	LEU A 318	242.040	-68.906	108.254	1.00	39.24	A
55	ATOM C	1545	C	LEU A 318	238.440	-68.952	111.425	1.00	41.79	A
	ATOM O	1546	O	LEU A 318	238.499	-67.943	112.191	1.00	36.26	A
60	ATOM N	1547	N	CYS A 319	237.301	-69.398	110.858	1.00	35.62	A
	ATOM C	1548	CA	CYS A 319	236.053	-68.700	111.024	1.00	40.61	A
	ATOM C	1549	CB	CYS A 319	235.013	-69.338	110.158	1.00	35.35	A

Atom	Seq	Res	Chain	X	Y	Z	Occ	B	Alt
ATOM S	1550	SG	CYS A 319	233.324	-68.489	110.215	1.00	25.40	A
ATOM C	1551	C	CYS A 319	235.640	-68.734	112.482	1.00	35.51	A
5 ATOM O	1552	O	CYS A 319	235.027	-67.810	112.980	1.00	40.27	A
ATOM N	1553	N	TYR A 320	236.009	-69.795	113.182	1.00	38.46	A
10 ATOM C	1554	CA	TYR A 320	235.683	-69.942	114.604	1.00	39.25	A
ATOM C	1555	CB	TYR A 320	235.867	-71.406	115.016	1.00	37.24	A
ATOM C	1556	CG	TYR A 320	235.634	-71.683	116.479	1.00	38.04	A
15 ATOM C	1557	CD1	TYR A 320	236.573	-71.333	117.438	1.00	34.91	A
ATOM C	1558	CE1	TYR A 320	236.380	-71.640	118.800	1.00	31.79	A
20 ATOM C	1559	CD2	TYR A 320	234.484	-72.331	116.892	1.00	39.29	A
ATOM C	1560	CE2	TYR A 320	234.248	-72.628	118.233	1.00	35.49	A
ATOM C	1561	CZ	TYR A 320	235.191	-72.289	119.198	1.00	41.97	A
25 ATOM O	1562	OH	TYR A 320	234.905	-72.575	120.532	1.00	35.00	A
ATOM C	1563	C	TYR A 320	236.613	-69.038	115.435	1.00	43.31	A
30 ATOM O	1564	O	TYR A 320	236.166	-68.318	116.322	1.00	51.83	A
ATOM N	1565	N	GLU A 321	237.910	-69.073	115.144	1.00	42.04	A
ATOM C	1566	CA	GLU A 321	238.860	-68.249	115.871	1.00	43.24	A
35 ATOM C	1567	CB	GLU A 321	240.273	-68.552	115.419	1.00	36.62	A
ATOM C	1568	CG	GLU A 321	241.311	-67.733	116.144	1.00	43.20	A
40 ATOM C	1569	CD	GLU A 321	242.689	-68.087	115.740	1.00	47.61	A
ATOM O	1570	OE1	GLU A 321	242.845	-69.101	115.003	1.00	49.19	A
ATOM O	1571	OE2	GLU A 321	243.606	-67.350	116.171	1.00	55.54	A
45 ATOM C	1572	C	GLU A 321	238.569	-66.763	115.714	1.00	42.47	A
ATOM O	1573	O	GLU A 321	238.794	-65.970	116.656	1.00	48.77	A
50 ATOM N	1574	N	PHE A 322	238.073	-66.377	114.539	1.00	40.79	A
ATOM C	1575	CA	PHE A 322	237.728	-64.970	114.299	1.00	37.96	A
ATOM C	1576	CB	PHE A 322	237.361	-64.737	112.846	1.00	37.47	A
55 ATOM C	1577	CG	PHE A 322	238.517	-64.880	111.892	1.00	39.59	A
ATOM C	1578	CD1	PHE A 322	239.839	-64.729	112.338	1.00	34.97	A
60 ATOM C	1579	CD2	PHE A 322	238.279	-65.133	110.515	1.00	41.97	A
ATOM C	1580	CE1	PHE A 322	240.892	-64.830	111.441	1.00	36.15	A

5	ATOM C	1581	CE2	PHE	A	322	239.342	-65.232	109.605	1.00	35.10	A
	ATOM C	1582	CZ	PHE	A	322	240.649	-65.081	110.070	1.00	38.47	A
	ATOM C	1583	C	PHE	A	322	236.569	-64.466	115.166	1.00	40.06	A
	ATOM O	1584	O	PHE	A	322	236.542	-63.305	115.532	1.00	37.07	A
10	ATOM N	1585	N	LEU	A	323	235.636	-65.356	115.499	1.00	34.80	A
	ATOM C	1586	CA	LEU	A	323	234.484	-65.021	116.291	1.00	30.32	A
15	ATOM C	1587	CB	LEU	A	323	233.317	-65.873	115.774	1.00	28.53	A
	ATOM C	1588	CG	LEU	A	323	232.935	-65.689	114.325	1.00	29.77	A
	ATOM C	1589	CD1	LEU	A	323	231.967	-66.804	113.984	1.00	24.59	A
20	ATOM C	1590	CD2	LEU	A	323	232.306	-64.288	114.046	1.00	30.36	A
	ATOM C	1591	C	LEU	A	323	234.661	-65.226	117.824	1.00	40.81	A
25	ATOM O	1592	O	LEU	A	323	234.058	-64.495	118.618	1.00	36.74	A
	ATOM N	1593	N	VAL	A	324	235.435	-66.247	118.216	1.00	38.37	A
30	ATOM C	1594	CA	VAL	A	324	235.629	-66.590	119.612	1.00	35.74	A
	ATOM C	1595	CB	VAL	A	324	235.648	-68.102	119.816	1.00	37.17	A
	ATOM C	1596	CG1	VAL	A	324	235.879	-68.419	121.294	1.00	34.96	A
35	ATOM C	1597	CG2	VAL	A	324	234.352	-68.697	119.303	1.00	26.08	A
	ATOM C	1598	C	VAL	A	324	236.903	-66.012	120.154	1.00	35.95	A
	ATOM O	1599	O	VAL	A	324	236.947	-65.631	121.301	1.00	44.11	A
40	ATOM N	1600	N	GLY	A	325	237.936	-65.929	119.330	1.00	41.01	A
	ATOM C	1601	CA	GLY	A	325	239.198	-65.355	119.782	1.00	39.51	A
	ATOM C	1602	C	GLY	A	325	240.283	-66.402	119.960	1.00	44.55	A
45	ATOM O	1603	O	GLY	A	325	241.414	-66.092	120.321	1.00	38.22	A
	ATOM N	1604	N	LYS	A	326	239.929	-67.663	119.722	1.00	45.05	A
50	ATOM C	1605	CA	LYS	A	326	240.881	-68.764	119.861	1.00	45.42	A
	ATOM C	1606	CB	LYS	A	326	240.994	-69.180	121.325	1.00	52.62	A
	ATOM C	1607	CG	LYS	A	326	239.699	-69.600	121.927	1.00	55.78	A
55	ATOM C	1608	CD	LYS	A	326	239.856	-69.912	123.415	1.00	60.70	A
	ATOM C	1609	CE	LYS	A	326	238.486	-70.233	124.058	1.00	66.17	A
60	ATOM N	1610	NZ	LYS	A	326	238.569	-70.651	125.479	1.00	62.77	A
	ATOM C	1611	C	LYS	A	326	240.419	-69.937	119.005	1.00	46.11	A

5	ATOM O	1612	O	LYS A 326	239.259	-70.074	118.767	1.00	39.63	A
	ATOM N	1613	N	PRO A 327	241.336	-70.820	118.568	1.00	53.36	A
	ATOM C	1614	CD	PRO A 327	242.773	-70.850	118.901	1.00	43.78	A
	ATOM C	1615	CA	PRO A 327	240.980	-71.968	117.726	1.00	41.74	A
10	ATOM C	1616	CB	PRO A 327	242.331	-72.631	117.446	1.00	38.86	A
	ATOM C	1617	CG	PRO A 327	243.349	-71.561	117.738	1.00	42.00	A
15	ATOM C	1618	C	PRO A 327	240.064	-72.895	118.474	1.00	40.42	A
	ATOM O	1619	O	PRO A 327	240.166	-73.021	119.700	1.00	46.66	A
	ATOM N	1620	N	PRO A 328	239.209	-73.624	117.743	1.00	40.91	A
20	ATOM C	1621	CD	PRO A 328	239.083	-73.540	116.278	1.00	35.93	A
	ATOM C	1622	CA	PRO A 328	238.232	-74.572	118.297	1.00	43.34	A
25	ATOM C	1623	CB	PRO A 328	237.340	-74.900	117.106	1.00	40.94	A
	ATOM C	1624	CG	PRO A 328	238.298	-74.799	115.948	1.00	38.83	A
	ATOM C	1625	C	PRO A 328	238.785	-75.820	118.933	1.00	44.48	A
30	ATOM O	1626	O	PRO A 328	238.075	-76.507	119.657	1.00	56.46	A
	ATOM N	1627	N	PHE A 329	240.053	-76.118	118.674	1.00	50.25	A
35	ATOM C	1628	CA	PHE A 329	240.691	-77.334	119.223	1.00	45.46	A
	ATOM C	1629	CB	PHE A 329	241.119	-78.268	118.089	1.00	42.34	A
	ATOM C	1630	CG	PHE A 329	240.026	-78.559	117.139	1.00	42.28	A
40	ATOM C	1631	CD1	PHE A 329	238.895	-79.252	117.575	1.00	39.79	A
	ATOM C	1632	CD2	PHE A 329	240.097	-78.138	115.808	1.00	39.80	A
45	ATOM C	1633	CE1	PHE A 329	237.824	-79.529	116.665	1.00	42.28	A
	ATOM C	1634	CE2	PHE A 329	239.034	-78.408	114.902	1.00	45.87	A
	ATOM C	1635	CZ	PHE A 329	237.903	-79.106	115.332	1.00	40.12	A
50	ATOM C	1636	C	PHE A 329	241.904	-76.978	120.064	1.00	45.73	A
	ATOM O	1637	O	PHE A 329	242.769	-77.808	120.277	1.00	40.30	A
55	ATOM N	1638	N	GLU A 330	241.958	-75.741	120.543	1.00	44.00	A
	ATOM C	1639	CA	GLU A 330	243.070	-75.285	121.345	1.00	50.19	A
	ATOM C	1640	CB	GLU A 330	242.855	-73.844	121.787	1.00	54.34	A
60	ATOM C	1641	CG	GLU A 330	244.140	-73.087	122.035	1.00	65.74	A
	ATOM C	1642	CD	GLU A 330	243.932	-71.802	122.845	1.00	74.00	A

5	ATOM O	1643	OE1	GLU	A	330	244.822	-70.906	122.794	1.00	80.13	A
	ATOM O	1644	OE2	GLU	A	330	242.884	-71.701	123.543	1.00	77.27	A
	ATOM C	1645	C	GLU	A	330	243.172	-76.161	122.550	1.00	51.87	A
	ATOM O	1646	O	GLU	A	330	242.158	-76.668	123.029	1.00	54.61	A
10	ATOM N	1647	N	ALA	A	331	244.404	-76.359	123.020	1.00	56.85	A
	ATOM C	1648	CA	ALA	A	331	244.680	-77.163	124.217	1.00	60.04	A
15	ATOM C	1649	CB	ALA	A	331	244.791	-78.618	123.872	1.00	51.13	A
	ATOM C	1650	C	ALA	A	331	245.992	-76.676	124.795	1.00	60.84	A
20	ATOM O	1651	O	ALA	A	331	246.630	-75.805	124.208	1.00	69.22	A
	ATOM N	1652	N	ASN	A	332	246.378	-77.197	125.962	1.00	64.86	A
	ATOM C	1653	CA	ASN	A	332	247.637	-76.790	126.560	1.00	61.08	A
	ATOM C	1654	CB	ASN	A	332	247.514	-76.742	128.100	1.00	60.00	A
25	ATOM C	1655	CG	ASN	A	332	246.822	-75.435	128.611	1.00	67.42	A
	ATOM O	1656	OD1	ASN	A	332	247.429	-74.359	128.654	1.00	68.56	A
30	ATOM N	1657	ND2	ASN	A	332	245.547	-75.544	129.000	1.00	72.60	A
	ATOM C	1658	C	ASN	A	332	248.807	-77.666	126.080	1.00	60.05	A
35	ATOM O	1659	O	ASN	A	332	249.966	-77.257	126.234	1.00	65.40	A
	ATOM N	1660	N	THR	A	333	248.512	-78.823	125.460	1.00	53.02	A
40	ATOM C	1661	CA	THR	A	333	249.562	-79.745	124.976	1.00	54.16	A
	ATOM C	1662	CB	THR	A	333	249.652	-81.103	125.782	1.00	55.23	A
	ATOM O	1663	OG1	THR	A	333	248.822	-82.111	125.160	1.00	53.00	A
	ATOM C	1664	CG2	THR	A	333	249.296	-80.907	127.225	1.00	55.86	A
45	ATOM C	1665	C	THR	A	333	249.400	-80.153	123.497	1.00	59.22	A
	ATOM O	1666	O	THR	A	333	248.379	-79.845	122.897	1.00	59.44	A
50	ATOM N	1667	N	TYR	A	334	250.358	-80.901	122.930	1.00	66.35	A
	ATOM C	1668	CA	TYR	A	334	250.331	-81.305	121.506	1.00	67.76	A
55	ATOM C	1669	CB	TYR	A	334	251.770	-81.458	120.999	1.00	65.59	A
	ATOM C	1670	CG	TYR	A	334	251.922	-82.193	119.636	1.00	60.98	A
60	ATOM C	1671	CD1	TYR	A	334	252.369	-81.519	118.539	1.00	58.37	A
	ATOM C	1672	CE1	TYR	A	334	252.454	-82.152	117.323	1.00	57.12	A
	ATOM C	1673	CD2	TYR	A	334	251.556	-83.561	119.454	1.00	60.46	A

5	ATOM C	1674	CE2	TYR	A	334	251.612	-84.203	118.235	1.00	54.51	A
	ATOM C	1675	CZ	TYR	A	334	252.081	-83.483	117.170	1.00	61.53	A
10	ATOM O	1676	OH	TYR	A	334	252.259	-84.054	115.932	1.00	64.63	A
	ATOM C	1677	C	TYR	A	334	249.706	-82.673	121.408	1.00	72.76	A
15	ATOM O	1678	O	TYR	A	334	249.561	-83.257	120.347	1.00	80.80	A
	ATOM N	1679	N	GLN	A	335	249.281	-83.198	122.511	1.00	75.82	A
20	ATOM C	1680	CA	GLN	A	335	248.849	-84.550	122.438	1.00	75.10	A
	ATOM C	1681	CB	GLN	A	335	249.822	-85.260	123.381	1.00	74.39	A
25	ATOM C	1682	CG	GLN	A	335	251.326	-84.889	123.021	1.00	71.11	A
	ATOM C	1683	CD	GLN	A	335	252.200	-84.301	124.134	1.00	70.17	A
30	ATOM O	1684	OE1	GLN	A	335	253.434	-84.204	123.959	1.00	71.56	A
	ATOM N	1685	NE2	GLN	A	335	251.605	-83.897	125.269	1.00	67.14	A
35	ATOM C	1686	C	GLN	A	335	247.415	-84.426	122.926	1.00	72.12	A
	ATOM O	1687	O	GLN	A	335	246.584	-85.314	122.698	1.00	70.11	A
40	ATOM N	1688	N	GLU	A	336	247.129	-83.272	123.527	1.00	67.17	A
	ATOM C	1689	CA	GLU	A	336	245.815	-82.981	124.050	1.00	66.23	A
45	ATOM C	1690	CB	GLU	A	336	245.911	-81.929	125.131	1.00	54.23	A
	ATOM C	1691	C	GLU	A	336	245.132	-82.389	122.779	1.00	63.60	A
50	ATOM O	1692	O	GLU	A	336	243.998	-82.726	122.478	1.00	68.92	A
	ATOM N	1693	N	THR	A	337	245.807	-81.474	122.060	1.00	63.51	A
55	ATOM C	1694	CA	THR	A	337	245.246	-80.840	120.863	1.00	45.32	A
	ATOM C	1695	CB	THR	A	337	246.221	-79.805	120.292	1.00	48.60	A
60	ATOM O	1696	OG1	THR	A	337	246.433	-78.730	121.227	1.00	44.49	A
	ATOM C	1697	CG2	THR	A	337	245.691	-79.262	118.948	1.00	33.80	A
65	ATOM C	1698	C	THR	A	337	245.031	-81.916	119.825	1.00	55.74	A
	ATOM O	1699	O	THR	A	337	244.036	-81.911	119.094	1.00	53.43	A
70	ATOM N	1700	N	TYR	A	338	245.979	-82.848	119.758	1.00	62.69	A
	ATOM C	1701	CA	TYR	A	338	245.902	-83.948	118.795	1.00	62.09	A
75	ATOM C	1702	CB	TYR	A	338	247.056	-84.923	119.028	1.00	70.33	A
	ATOM C	1703	CG	TYR	A	338	247.098	-86.080	118.034	1.00	74.69	A
80	ATOM C	1704	CD1	TYR	A	338	248.041	-86.116	117.016	1.00	72.79	A

5	ATOM C	1705	CE1	TYR	A	338	248.050	-87.154	116.101	1.00	75.92	A
	ATOM C	1706	CD2	TYR	A	338	246.167	-87.121	118.096	1.00	70.94	A
	ATOM C	1707	CE2	TYR	A	338	246.167	-88.153	117.173	1.00	73.14	A
	ATOM C	1708	CZ	TYR	A	338	247.102	-88.168	116.186	1.00	73.24	A
10	ATOM O	1709	OH	TYR	A	338	247.091	-89.196	115.273	1.00	74.46	A
	ATOM C	1710	C	TYR	A	338	244.586	-84.698	118.971	1.00	62.03	A
	ATOM O	1711	O	TYR	A	338	243.884	-85.017	117.982	1.00	52.46	A
15	ATOM N	1712	N	LYS	A	339	244.267	-84.991	120.242	1.00	58.53	A
	ATOM C	1713	CA	LYS	A	339	243.048	-85.733	120.587	1.00	51.87	A
20	ATOM C	1714	CB	LYS	A	339	243.020	-86.042	122.063	1.00	52.84	A
	ATOM C	1715	C	LYS	A	339	241.791	-84.990	120.165	1.00	50.97	A
25	ATOM O	1716	O	LYS	A	339	240.975	-85.531	119.412	1.00	50.87	A
	ATOM N	1717	N	ARG	A	340	241.675	-83.725	120.575	1.00	44.05	A
30	ATOM C	1718	CA	ARG	A	340	240.507	-82.938	120.230	1.00	47.22	A
	ATOM C	1719	CB	ARG	A	340	240.532	-81.574	120.904	1.00	45.76	A
	ATOM C	1720	CG	ARG	A	340	240.286	-81.607	122.398	1.00	52.85	A
35	ATOM C	1721	CD	ARG	A	340	240.241	-80.202	122.999	1.00	59.79	A
	ATOM N	1722	NE	ARG	A	340	239.045	-79.491	122.535	1.00	67.64	A
	ATOM C	1723	CZ	ARG	A	340	238.843	-78.186	122.672	1.00	65.86	A
40	ATOM N	1724	NH1	ARG	A	340	239.763	-77.446	123.254	1.00	67.71	A
	ATOM N	1725	NH2	ARG	A	340	237.722	-77.631	122.240	1.00	68.60	A
45	ATOM C	1726	C	ARG	A	340	240.299	-82.765	118.738	1.00	46.20	A
	ATOM O	1727	O	ARG	A	340	239.144	-82.785	118.274	1.00	48.74	A
	ATOM N	1728	N	ILE	A	341	241.387	-82.597	117.979	1.00	47.52	A
50	ATOM C	1729	CA	ILE	A	341	241.253	-82.462	116.511	1.00	49.01	A
	ATOM C	1730	CB	ILE	A	341	242.586	-82.067	115.787	1.00	48.35	A
55	ATOM C	1731	CG2	ILE	A	341	242.367	-82.130	114.290	1.00	34.18	A
	ATOM C	1732	CG1	ILE	A	341	243.053	-80.674	116.236	1.00	44.80	A
	ATOM C	1733	CD1	ILE	A	341	244.317	-80.259	115.592	1.00	47.34	A
60	ATOM C	1734	C	ILE	A	341	240.783	-83.752	115.851	1.00	53.55	A
	ATOM O	1735	O	ILE	A	341	239.936	-83.734	114.948	1.00	44.79	A

5	ATOM N	1736	N	SER A 342	241.369	-84.867	116.286	1.00	59.31	A
	ATOM C	1737	CA	SER A 342	241.014	-86.175	115.743	1.00	65.95	A
	ATOM C	1738	CB	SER A 342	242.037	-87.227	116.158	1.00	66.33	A
	ATOM O	1739	OG	SER A 342	241.613	-88.516	115.745	1.00	63.35	A
10	ATOM C	1740	C	SER A 342	239.628	-86.604	116.202	1.00	65.99	A
	ATOM O	1741	O	SER A 342	238.941	-87.327	115.475	1.00	61.18	A
15	ATOM N	1742	N	ARG A 343	239.232	-86.162	117.400	1.00	61.34	A
	ATOM C	1743	CA	ARG A 343	237.910	-86.478	117.932	1.00	59.46	A
	ATOM C	1744	CB	ARG A 343	237.888	-86.410	119.456	1.00	58.77	A
20	ATOM C	1745	CG	ARG A 343	238.466	-87.604	120.201	1.00	47.50	A
	ATOM C	1746	CD	ARG A 343	238.360	-87.314	121.675	1.00	60.64	A
25	ATOM N	1747	NE	ARG A 343	238.972	-88.327	122.530	1.00	66.55	A
	ATOM C	1748	CZ	ARG A 343	238.930	-88.278	123.865	1.00	74.36	A
	ATOM N	1749	NH1	ARG A 343	238.309	-87.268	124.510	1.00	73.84	A
30	ATOM N	1750	NH2	ARG A 343	239.502	-89.248	124.573	1.00	82.35	A
	ATOM C	1751	C	ARG A 343	236.902	-85.448	117.406	1.00	62.95	A
35	ATOM O	1752	O	ARG A 343	235.682	-85.706	117.372	1.00	61.25	A
	ATOM N	1753	N	VAL A 344	237.421	-84.275	117.011	1.00	62.37	A
	ATOM C	1754	CA	VAL A 344	236.592	-83.163	116.517	1.00	52.53	A
40	ATOM C	1755	CB	VAL A 344	235.625	-83.614	115.386	1.00	46.83	A
	ATOM C	1756	CG1	VAL A 344	235.005	-82.383	114.685	1.00	30.17	A
45	ATOM C	1757	CG2	VAL A 344	236.378	-84.445	114.375	1.00	41.05	A
	ATOM C	1758	C	VAL A 344	235.794	-82.735	117.737	1.00	56.35	A
	ATOM O	1759	O	VAL A 344	234.569	-82.790	117.750	1.00	58.20	A
50	ATOM N	1760	N	GLU A 345	236.521	-82.345	118.775	1.00	52.70	A
	ATOM C	1761	CA	GLU A 345	235.945	-81.929	120.037	1.00	55.50	A
55	ATOM C	1762	CB	GLU A 345	236.726	-82.610	121.170	1.00	59.39	A
	ATOM C	1763	CG	GLU A 345	236.049	-82.656	122.512	1.00	70.94	A
	ATOM C	1764	CD	GLU A 345	236.741	-83.623	123.456	1.00	80.37	A
60	ATOM O	1765	OE1	GLU A 345	236.904	-84.815	123.076	1.00	83.68	A
	ATOM O	1766	OE2	GLU A 345	237.114	-83.190	124.572	1.00	84.85	A

Line	Atom	Res	Chain	ResID	X	Y	Z	Occup	B-factor	Alt
5	ATOM C	1767	C	GLU A 345	235.984	-80.414	120.226	1.00	55.94	A
	ATOM O	1768	O	GLU A 345	237.012	-79.866	120.647	1.00	52.34	A
	ATOM N	1769	N	PHE A 346	234.868	-79.746	119.941	1.00	55.31	A
	ATOM C	1770	CA	PHE A 346	234.777	-78.298	120.123	1.00	58.97	A
10	ATOM C	1771	CB	PHE A 346	235.238	-77.601	118.840	1.00	55.59	A
	ATOM C	1772	CG	PHE A 346	234.247	-77.671	117.721	1.00	51.30	A
	ATOM C	1773	CD1	PHE A 346	233.315	-76.667	117.540	1.00	47.92	A
15	ATOM C	1774	CD2	PHE A 346	234.261	-78.734	116.842	1.00	51.74	A
	ATOM C	1775	CE1	PHE A 346	232.396	-76.715	116.483	1.00	54.03	A
20	ATOM C	1776	CE2	PHE A 346	233.348	-78.810	115.764	1.00	54.32	A
	ATOM C	1777	CZ	PHE A 346	232.409	-77.803	115.575	1.00	51.48	A
	ATOM C	1778	C	PHE A 346	233.356	-77.832	120.501	1.00	60.04	A
25	ATOM O	1779	O	PHE A 346	232.368	-78.494	120.173	1.00	69.92	A
	ATOM N	1780	N	THR A 347	233.261	-76.697	121.184	1.00	56.17	A
30	ATOM C	1781	CA	THR A 347	231.979	-76.158	121.555	1.00	54.44	A
	ATOM C	1782	CB	THR A 347	231.732	-76.329	123.013	1.00	47.09	A
	ATOM O	1783	OG1	THR A 347	232.718	-75.600	123.725	1.00	47.43	A
35	ATOM C	1784	CG2	THR A 347	231.799	-77.783	123.402	1.00	48.24	A
	ATOM C	1785	C	THR A 347	231.885	-74.683	121.223	1.00	56.33	A
40	ATOM O	1786	O	THR A 347	232.902	-73.985	121.113	1.00	62.80	A
	ATOM N	1787	N	PHE A 348	230.646	-74.235	120.999	1.00	63.69	A
45	ATOM C	1788	CA	PHE A 348	230.389	-72.815	120.723	1.00	65.89	A
	ATOM C	1789	CB	PHE A 348	229.306	-72.558	119.708	1.00	57.72	A
	ATOM C	1790	CG	PHE A 348	229.584	-73.148	118.381	1.00	55.81	A
50	ATOM C	1791	CD1	PHE A 348	229.017	-74.364	118.020	1.00	51.99	A
	ATOM C	1792	CD2	PHE A 348	230.337	-72.462	117.450	1.00	53.67	A
	ATOM C	1793	CE1	PHE A 348	229.171	-74.857	116.780	1.00	46.52	A
55	ATOM C	1794	CE2	PHE A 348	230.492	-72.966	116.190	1.00	50.86	A
	ATOM C	1795	CZ	PHE A 348	229.903	-74.166	115.860	1.00	51.38	A
60	ATOM C	1796	C	PHE A 348	229.966	-72.048	121.961	1.00	65.81	A
	ATOM O	1797	O	PHE A 348	229.223	-72.532	122.808	1.00	73.51	A

5	ATOM N	1798	N	PRO	A	349	230.578	-70.898	122.150	1.00	59.06	A
	ATOM C	1799	CD	PRO	A	349	232.018	-71.026	121.861	1.00	61.27	A
	ATOM C	1800	CA	PRO	A	349	230.381	-69.933	123.199	1.00	56.66	A
	ATOM C	1801	CB	PRO	A	349	231.466	-68.944	122.870	1.00	58.77	A
10	ATOM C	1802	CG	PRO	A	349	232.627	-69.875	122.485	1.00	55.14	A
	ATOM C	1803	C	PRO	A	349	228.929	-69.409	122.948	1.00	57.97	A
15	ATOM O	1804	O	PRO	A	349	228.312	-69.642	121.916	1.00	59.47	A
	ATOM N	1805	N	ASP	A	350	228.344	-68.735	123.909	1.00	59.19	A
	ATOM C	1806	CA	ASP	A	350	226.961	-68.282	123.714	1.00	51.98	A
20	ATOM C	1807	CB	ASP	A	350	226.338	-67.819	125.044	1.00	65.27	A
	ATOM C	1808	CG	ASP	A	350	226.140	-68.958	126.020	1.00	72.68	A
25	ATOM O	1809	OD1	ASP	A	350	225.764	-68.668	127.188	1.00	77.91	A
	ATOM O	1810	OD2	ASP	A	350	226.359	-70.131	125.607	1.00	78.14	A
	ATOM C	1811	C	ASP	A	350	226.787	-67.197	122.665	1.00	54.69	A
30	ATOM O	1812	O	ASP	A	350	225.753	-67.202	121.947	1.00	40.28	A
	ATOM N	1813	N	PHE	A	351	227.786	-66.308	122.539	1.00	47.45	A
35	ATOM C	1814	CA	PHE	A	351	227.682	-65.217	121.584	1.00	51.83	A
	ATOM C	1815	CB	PHE	A	351	228.693	-64.106	121.893	1.00	48.14	A
	ATOM C	1816	CG	PHE	A	351	230.108	-64.580	122.004	1.00	51.21	A
40	ATOM C	1817	CD1	PHE	A	351	230.589	-65.111	123.207	1.00	49.73	A
	ATOM C	1818	CD2	PHE	A	351	230.979	-64.468	120.915	1.00	46.79	A
45	ATOM C	1819	CE1	PHE	A	351	231.906	-65.506	123.312	1.00	48.51	A
	ATOM C	1820	CE2	PHE	A	351	232.294	-64.864	121.026	1.00	47.18	A
	ATOM C	1821	CZ	PHE	A	351	232.758	-65.379	122.215	1.00	45.61	A
50	ATOM C	1822	C	PHE	A	351	227.797	-65.610	120.125	1.00	52.56	A
	ATOM O	1823	O	PHE	A	351	227.604	-64.771	119.250	1.00	57.29	A
55	ATOM N	1824	N	VAL	A	352	228.115	-66.874	119.863	1.00	54.95	A
	ATOM C	1825	CA	VAL	A	352	228.263	-67.341	118.495	1.00	48.00	A
	ATOM C	1826	CB	VAL	A	352	229.145	-68.621	118.432	1.00	43.19	A
60	ATOM C	1827	CG1	VAL	A	352	229.300	-69.094	117.035	1.00	33.61	A
	ATOM C	1828	CG2	VAL	A	352	230.509	-68.325	118.972	1.00	39.08	A

5	ATOM C	1829	C	VAL A	352	226.875	-67.603	117.916	1.00	48.25	A
	ATOM O	1830	O	VAL A	352	226.211	-68.567	118.255	1.00	51.46	A
	ATOM N	1831	N	THR A	353	226.446	-66.748	117.004	1.00	47.51	A
	ATOM C	1832	CA	THR A	353	225.122	-66.886	116.413	1.00	53.02	A
10	ATOM C	1833	CB	THR A	353	224.844	-65.817	115.383	1.00	47.94	A
	ATOM O	1834	OG1	THR A	353	225.671	-66.052	114.246	1.00	54.22	A
15	ATOM C	1835	CG2	THR A	353	225.130	-64.437	115.950	1.00	47.89	A
	ATOM C	1836	C	THR A	353	224.908	-68.227	115.753	1.00	52.60	A
20	ATOM O	1837	O	THR A	353	225.851	-68.974	115.552	1.00	52.94	A
	ATOM N	1838	N	GLU A	354	223.654	-68.513	115.404	1.00	55.25	A
	ATOM C	1839	CA	GLU A	354	223.259	-69.786	114.819	1.00	56.40	A
	ATOM C	1840	CB	GLU A	354	221.736	-69.929	114.829	1.00	53.45	A
25	ATOM C	1841	C	GLU A	354	223.762	-69.866	113.416	1.00	56.12	A
	ATOM O	1842	O	GLU A	354	224.078	-70.954	112.927	1.00	62.85	A
30	ATOM N	1843	N	GLY A	355	223.831	-68.718	112.749	1.00	61.99	A
	ATOM C	1844	CA	GLY A	355	224.317	-68.699	111.373	1.00	52.27	A
35	ATOM C	1845	C	GLY A	355	225.787	-69.093	111.250	1.00	52.90	A
	ATOM O	1846	O	GLY A	355	226.166	-69.822	110.327	1.00	47.53	A
40	ATOM N	1847	N	ALA A	356	226.611	-68.602	112.182	1.00	47.86	A
	ATOM C	1848	CA	ALA A	356	228.022	-68.912	112.199	1.00	45.96	A
	ATOM C	1849	CB	ALA A	356	228.721	-67.995	113.123	1.00	42.05	A
	ATOM C	1850	C	ALA A	356	228.221	-70.359	112.627	1.00	47.72	A
45	ATOM O	1851	O	ALA A	356	229.011	-71.078	112.025	1.00	46.93	A
	ATOM N	1852	N	ARG A	357	227.486	-70.784	113.651	1.00	49.03	A
50	ATOM C	1853	CA	ARG A	357	227.558	-72.153	114.146	1.00	56.76	A
	ATOM C	1854	CB	ARG A	357	226.549	-72.374	115.280	1.00	55.71	A
55	ATOM C	1855	CG	ARG A	357	226.876	-71.606	116.583	1.00	57.21	A
	ATOM C	1856	CD	ARG A	357	226.018	-72.108	117.752	1.00	41.40	A
60	ATOM N	1857	NE	ARG A	357	226.260	-71.310	118.928	1.00	43.14	A
	ATOM C	1858	CZ	ARG A	357	225.979	-71.698	120.148	1.00	39.58	A
	ATOM N	1859	NH1	ARG A	357	225.456	-72.893	120.340	1.00	42.66	A

5	ATOM N	1860	NH2	ARG	A	357	226.191	-70.869	121.163	1.00	51.41	A
	ATOM C	1861	C	ARG	A	357	227.299	-73.181	113.043	1.00	58.61	A
	ATOM O	1862	O	ARG	A	357	227.922	-74.260	112.996	1.00	62.70	A
	ATOM N	1863	N	ASP	A	358	226.383	-72.845	112.150	1.00	56.80	A
10	ATOM C	1864	CA	ASP	A	358	226.053	-73.738	111.055	1.00	56.49	A
	ATOM C	1865	CB	ASP	A	358	224.792	-73.245	110.363	1.00	59.12	A
	ATOM C	1866	CG	ASP	A	358	224.380	-74.141	109.209	1.00	65.41	A
15	ATOM O	1867	OD1	ASP	A	358	224.036	-75.319	109.461	1.00	60.89	A
	ATOM O	1868	OD2	ASP	A	358	224.403	-73.669	108.049	1.00	68.71	A
20	ATOM C	1869	C	ASP	A	358	227.178	-73.837	110.017	1.00	56.31	A
	ATOM O	1870	O	ASP	A	358	227.523	-74.915	109.545	1.00	56.62	A
25	ATOM N	1871	N	LEU	A	359	227.735	-72.694	109.640	1.00	57.58	A
	ATOM C	1872	CA	LEU	A	359	228.812	-72.663	108.658	1.00	55.45	A
	ATOM C	1873	CB	LEU	A	359	229.158	-71.227	108.302	1.00	53.49	A
30	ATOM C	1874	CG	LEU	A	359	230.326	-71.029	107.344	1.00	49.10	A
	ATOM C	1875	CD1	LEU	A	359	230.077	-71.756	106.082	1.00	42.56	A
35	ATOM C	1876	CD2	LEU	A	359	230.525	-69.538	107.083	1.00	51.15	A
	ATOM C	1877	C	LEU	A	359	230.048	-73.366	109.200	1.00	57.66	A
	ATOM O	1878	O	LEU	A	359	230.680	-74.142	108.481	1.00	65.55	A
40	ATOM N	1879	N	ILE	A	360	230.370	-73.121	110.470	1.00	49.19	A
	ATOM C	1880	CA	ILE	A	360	231.535	-73.740	111.089	1.00	43.07	A
45	ATOM C	1881	CB	ILE	A	360	231.819	-73.111	112.485	1.00	35.85	A
	ATOM C	1882	CG2	ILE	A	360	232.892	-73.858	113.220	1.00	37.90	A
	ATOM C	1883	CG1	ILE	A	360	232.254	-71.652	112.301	1.00	32.36	A
50	ATOM C	1884	CD1	ILE	A	360	232.250	-70.839	113.653	1.00	27.28	A
	ATOM C	1885	C	ILE	A	360	231.368	-75.240	111.229	1.00	40.84	A
55	ATOM O	1886	O	ILE	A	360	232.330	-75.980	111.042	1.00	44.75	A
	ATOM N	1887	N	SER	A	361	230.158	-75.670	111.591	1.00	46.60	A
	ATOM C	1888	CA	SER	A	361	229.855	-77.089	111.780	1.00	52.65	A
60	ATOM C	1889	CB	SER	A	361	228.546	-77.265	112.526	1.00	49.78	A
	ATOM O	1890	OG	SER	A	361	228.742	-77.062	113.925	1.00	60.97	A

	ATOM C	1891	C	SER A 361	229.827	-77.906	110.497	1.00	53.49	A
	ATOM O	1892	O	SER A 361	229.885	-79.159	110.538	1.00	53.09	A
5	ATOM N	1893	N	ARG A 362	229.799	-77.198	109.368	1.00	54.39	A
	ATOM C	1894	CA	ARG A 362	229.796	-77.841	108.066	1.00	52.12	A
10	ATOM C	1895	CB	ARG A 362	229.033	-76.978	107.065	1.00	59.93	A
	ATOM C	1896	CG	ARG A 362	227.535	-76.862	107.327	1.00	61.75	A
	ATOM C	1897	CD	ARG A 362	226.887	-75.820	106.401	1.00	69.51	A
15	ATOM N	1898	NE	ARG A 362	225.432	-75.784	106.547	1.00	76.19	A
	ATOM C	1899	CZ	ARG A 362	224.625	-76.795	106.216	1.00	80.23	A
20	ATOM N	1900	NH1	ARG A 362	225.128	-77.919	105.716	1.00	81.25	A
	ATOM N	1901	NH2	ARG A 362	223.313	-76.697	106.397	1.00	77.76	A
	ATOM C	1902	C	ARG A 362	231.211	-78.066	107.537	1.00	49.26	A
25	ATOM O	1903	O	ARG A 362	231.460	-79.036	106.822	1.00	49.03	A
	ATOM N	1904	N	LEU A 363	232.120	-77.162	107.891	1.00	49.05	A
30	ATOM C	1905	CA	LEU A 363	233.493	-77.234	107.438	1.00	46.81	A
	ATOM C	1906	CB	LEU A 363	234.134	-75.850	107.508	1.00	42.60	A
	ATOM C	1907	CG	LEU A 363	233.457	-74.729	106.714	1.00	44.53	A
35	ATOM C	1908	CD1	LEU A 363	234.050	-73.356	107.133	1.00	43.18	A
	ATOM C	1909	CD2	LEU A 363	233.602	-74.961	105.258	1.00	42.47	A
40	ATOM C	1910	C	LEU A 363	234.270	-78.228	108.280	1.00	49.03	A
	ATOM O	1911	O	LEU A 363	235.049	-79.020	107.751	1.00	57.90	A
	ATOM N	1912	N	LEU A 364	234.062	-78.186	109.589	1.00	47.92	A
45	ATOM C	1913	CA	LEU A 364	234.774	-79.071	110.488	1.00	49.66	A
	ATOM C	1914	CB	LEU A 364	234.792	-78.462	111.909	1.00	46.24	A
50	ATOM C	1915	CG	LEU A 364	235.511	-77.115	112.043	1.00	47.59	A
	ATOM C	1916	CD1	LEU A 364	235.230	-76.547	113.413	1.00	44.59	A
	ATOM C	1917	CD2	LEU A 364	237.029	-77.318	111.836	1.00	45.40	A
55	ATOM C	1918	C	LEU A 364	234.233	-80.493	110.526	1.00	50.53	A
	ATOM O	1919	O	LEU A 364	233.804	-80.963	111.575	1.00	56.94	A
60	ATOM N	1920	N	LYS A 365	234.267	-81.178	109.385	1.00	61.00	A
	ATOM C	1921	CA	LYS A 365	233.796	-82.564	109.263	1.00	64.52	A

5	ATOM C	1922	CB	LYS A 365	233.059	-82.728	107.925	1.00	60.48	A
	ATOM C	1923	CG	LYS A 365	231.753	-81.921	107.829	1.00	53.27	A
	ATOM C	1924	CD	LYS A 365	230.702	-82.412	108.828	1.00	61.58	A
	ATOM C	1925	CE	LYS A 365	229.295	-81.895	108.447	1.00	59.92	A
	ATOM N	1926	NZ	LYS A 365	228.297	-82.223	109.508	1.00	75.42	A
10	ATOM C	1927	C	LYS A 365	235.026	-83.500	109.392	1.00	66.56	A
	ATOM O	1928	O	LYS A 365	236.146	-83.084	109.123	1.00	71.71	A
	ATOM N	1929	N	HIS A 366	234.844	-84.748	109.813	1.00	68.20	A
	ATOM C	1930	CA	HIS A 366	236.011	-85.628	110.015	1.00	67.59	A
	ATOM C	1931	CB	HIS A 366	235.781	-86.664	111.109	1.00	66.12	A
20	ATOM C	1932	CG	HIS A 366	236.913	-87.628	111.242	1.00	68.47	A
	ATOM C	1933	CD2	HIS A 366	237.810	-87.749	112.245	1.00	66.88	A
	ATOM N	1934	ND1	HIS A 366	237.332	-88.487	110.238	1.00	66.01	A
	ATOM C	1935	CE1	HIS A 366	238.454	-89.075	110.623	1.00	70.20	A
	ATOM N	1936	NE2	HIS A 366	238.761	-88.643	111.832	1.00	64.97	A
30	ATOM C	1937	C	HIS A 366	236.184	-86.385	108.739	1.00	68.25	A
	ATOM O	1938	O	HIS A 366	237.098	-87.249	108.572	1.00	74.87	A
	ATOM N	1939	N	ASN A 367	235.262	-86.111	107.848	1.00	65.45	A
	ATOM C	1940	CA	ASN A 367	235.379	-86.795	106.656	1.00	62.81	A
	ATOM C	1941	CB	ASN A 367	234.189	-87.664	106.498	1.00	64.61	A
40	ATOM C	1942	CG	ASN A 367	234.335	-88.548	105.333	1.00	69.77	A
	ATOM O	1943	OD1	ASN A 367	234.339	-88.071	104.175	1.00	65.35	A
	ATOM N	1944	ND2	ASN A 367	234.518	-89.855	105.596	1.00	69.27	A
	ATOM C	1945	C	ASN A 367	235.504	-85.791	105.596	1.00	60.17	A
	ATOM O	1946	O	ASN A 367	234.685	-84.923	105.475	1.00	67.65	A
50	ATOM N	1947	N	PRO A 368	236.650	-85.797	104.923	1.00	60.54	A
	ATOM C	1948	CD	PRO A 368	237.882	-86.364	105.504	1.00	55.35	A
	ATOM C	1949	CA	PRO A 368	236.981	-84.895	103.820	1.00	55.82	A
	ATOM C	1950	CB	PRO A 368	238.199	-85.537	103.245	1.00	50.93	A
	ATOM C	1951	CG	PRO A 368	238.938	-85.936	104.468	1.00	54.85	A
60	ATOM C	1952	C	PRO A 368	235.870	-84.741	102.783	1.00	59.90	A

5	ATOM O	1953	O	PRO A 368	235.706	-83.658	102.240	1.00	61.00	A
	ATOM N	1954	N	SER A 369	235.093	-85.805	102.557	1.00	69.67	A
	ATOM C	1955	CA	SER A 369	234.000	-85.800	101.588	1.00	72.88	A
	ATOM C	1956	CB	SER A 369	233.537	-87.237	101.347	1.00	75.22	A
10	ATOM O	1957	OG	SER A 369	234.654	-88.115	101.256	1.00	85.92	A
	ATOM C	1958	C	SER A 369	232.810	-84.951	102.046	1.00	71.84	A
15	ATOM O	1959	O	SER A 369	232.217	-84.231	101.229	1.00	75.53	A
	ATOM N	1960	N	GLN A 370	232.465	-85.039	103.333	1.00	67.85	A
20	ATOM C	1961	CA	GLN A 370	231.339	-84.296	103.865	1.00	62.69	A
	ATOM C	1962	CB	GLN A 370	231.067	-84.743	105.296	1.00	64.15	A
	ATOM C	1963	CG	GLN A 370	230.629	-86.190	105.390	1.00	65.40	A
	ATOM C	1964	CD	GLN A 370	230.923	-86.768	106.745	1.00	69.41	A
25	ATOM O	1965	OE1	GLN A 370	230.904	-86.051	107.752	1.00	75.34	A
	ATOM N	1966	NE2	GLN A 370	231.189	-88.073	106.792	1.00	63.71	A
30	ATOM C	1967	C	GLN A 370	231.551	-82.778	103.799	1.00	63.34	A
	ATOM O	1968	O	GLN A 370	230.582	-82.028	103.608	1.00	65.90	A
35	ATOM N	1969	N	ARG A 371	232.802	-82.324	103.934	1.00	56.18	A
	ATOM C	1970	CA	ARG A 371	233.085	-80.905	103.889	1.00	54.33	A
	ATOM C	1971	CB	ARG A 371	234.581	-80.691	103.961	1.00	48.64	A
40	ATOM C	1972	CG	ARG A 371	235.109	-80.785	105.354	1.00	46.61	A
	ATOM C	1973	CD	ARG A 371	236.618	-80.922	105.403	1.00	43.30	A
45	ATOM N	1974	NE	ARG A 371	236.988	-81.971	106.350	1.00	42.51	A
	ATOM C	1975	CZ	ARG A 371	238.208	-82.476	106.436	1.00	42.45	A
	ATOM N	1976	NH1	ARG A 371	239.165	-81.997	105.635	1.00	36.24	A
50	ATOM N	1977	NH2	ARG A 371	238.449	-83.494	107.266	1.00	33.74	A
	ATOM C	1978	C	ARG A 371	232.496	-80.275	102.651	1.00	56.25	A
55	ATOM O	1979	O	ARG A 371	232.578	-80.836	101.587	1.00	64.77	A
	ATOM N	1980	N	PRO A 372	231.885	-79.089	102.783	1.00	60.04	A
60	ATOM C	1981	CD	PRO A 372	231.813	-78.305	104.029	1.00	57.31	A
	ATOM C	1982	CA	PRO A 372	231.260	-78.365	101.659	1.00	57.19	A
	ATOM C	1983	CB	PRO A 372	230.522	-77.231	102.348	1.00	55.89	A

5	ATOM C	1984	CG	PRO A	372	231.448	-76.927	103.522	1.00	60.48	A
	ATOM C	1985	C	PRO A	372	232.227	-77.848	100.593	1.00	59.74	A
10	ATOM O	1986	O	PRO A	372	233.424	-77.896	100.753	1.00	60.73	A
	ATOM N	1987	N	MET A	373	231.685	-77.356	99.497	1.00	66.48	A
15	ATOM C	1988	CA	MET A	373	232.482	-76.838	98.412	1.00	72.53	A
	ATOM C	1989	CB	MET A	373	231.763	-77.051	97.082	1.00	78.23	A
20	ATOM C	1990	CG	MET A	373	232.541	-77.969	96.165	1.00	91.60	A
	ATOM S	1991	SD	MET A	373	231.857	-78.033	94.463	1.00	92.28	A
25	ATOM C	1992	CE	MET A	373	230.337	-78.924	94.769	1.00	97.23	A
	ATOM C	1993	C	MET A	373	232.631	-75.339	98.682	1.00	69.48	A
30	ATOM O	1994	O	MET A	373	231.861	-74.740	99.424	1.00	71.05	A
	ATOM N	1995	N	LEU A	374	233.618	-74.722	98.060	1.00	66.97	A
35	ATOM C	1996	CA	LEU A	374	233.847	-73.303	98.261	1.00	65.90	A
	ATOM C	1997	CB	LEU A	374	235.155	-72.857	97.562	1.00	58.73	A
40	ATOM C	1998	CG	LEU A	374	236.446	-73.311	98.258	1.00	51.64	A
	ATOM C	1999	CD1	LEU A	374	237.625	-73.104	97.321	1.00	47.33	A
45	ATOM C	2000	CD2	LEU A	374	236.629	-72.531	99.548	1.00	52.27	A
	ATOM C	2001	C	LEU A	374	232.660	-72.469	97.798	1.00	67.13	A
50	ATOM O	2002	O	LEU A	374	232.500	-71.320	98.219	1.00	75.20	A
	ATOM N	2003	N	ARG A	375	231.814	-73.025	96.939	1.00	67.09	A
55	ATOM C	2004	CA	ARG A	375	230.654	-72.254	96.482	1.00	63.14	A
	ATOM C	2005	CB	ARG A	375	230.122	-72.780	95.162	1.00	60.43	A
60	ATOM C	2006	C	ARG A	375	229.561	-72.275	97.541	1.00	63.36	A
	ATOM O	2007	O	ARG A	375	228.882	-71.261	97.734	1.00	64.17	A
65	ATOM N	2008	N	GLU A	376	229.413	-73.397	98.245	1.00	56.91	A
	ATOM C	2009	CA	GLU A	376	228.404	-73.501	99.306	1.00	64.22	A
70	ATOM C	2010	CB	GLU A	376	228.314	-74.947	99.815	1.00	67.11	A
	ATOM C	2011	CG	GLU A	376	227.797	-75.921	98.783	1.00	81.78	A
75	ATOM C	2012	CD	GLU A	376	228.016	-77.372	99.187	1.00	87.25	A
	ATOM O	2013	OE1	GLU A	376	229.137	-77.887	98.974	1.00	95.99	A
	ATOM O	2014	OE2	GLU A	376	227.073	-78.001	99.732	1.00	98.67	A

5	ATOM C	2015	C	GLU A 376	228.791	-72.562	100.461	1.00	61.59	A
	ATOM O	2016	O	GLU A 376	227.950	-72.145	101.275	1.00	63.73	A
	ATOM N	2017	N	VAL A 377	230.078	-72.229	100.505	1.00	60.90	A
	ATOM C	2018	CA	VAL A 377	230.605	-71.361	101.539	1.00	60.11	A
10	ATOM C	2019	CB	VAL A 377	232.149	-71.606	101.780	1.00	57.13	A
	ATOM C	2020	CG1	VAL A 377	232.701	-70.591	102.788	1.00	52.18	A
15	ATOM C	2021	CG2	VAL A 377	232.364	-72.987	102.341	1.00	51.22	A
	ATOM C	2022	C	VAL A 377	230.354	-69.928	101.140	1.00	59.92	A
	ATOM O	2023	O	VAL A 377	229.915	-69.114	101.952	1.00	69.33	A
20	ATOM N	2024	N	LEU A 378	230.639	-69.625	99.884	1.00	54.97	A
	ATOM C	2025	CA	LEU A 378	230.466	-68.269	99.384	1.00	57.61	A
25	ATOM C	2026	CB	LEU A 378	231.178	-68.090	98.026	1.00	55.37	A
	ATOM C	2027	CG	LEU A 378	232.564	-67.442	97.937	1.00	56.77	A
30	ATOM C	2028	CD1	LEU A 378	232.986	-66.902	99.309	1.00	59.47	A
	ATOM C	2029	CD2	LEU A 378	233.517	-68.445	97.421	1.00	52.34	A
	ATOM C	2030	C	LEU A 378	228.995	-67.925	99.248	1.00	53.77	A
35	ATOM O	2031	O	LEU A 378	228.626	-66.775	99.062	1.00	56.35	A
	ATOM N	2032	N	GLU A 379	228.144	-68.930	99.367	1.00	58.84	A
40	ATOM C	2033	CA	GLU A 379	226.708	-68.714	99.236	1.00	63.13	A
	ATOM C	2034	CB	GLU A 379	226.101	-69.720	98.274	1.00	65.30	A
	ATOM C	2035	CG	GLU A 379	226.567	-69.569	96.831	1.00	70.53	A
45	ATOM C	2036	CD	GLU A 379	225.831	-70.533	95.895	1.00	76.21	A
	ATOM O	2037	OE1	GLU A 379	225.546	-71.692	96.329	1.00	70.09	A
50	ATOM O	2038	OE2	GLU A 379	225.547	-70.124	94.737	1.00	76.09	A
	ATOM C	2039	C	GLU A 379	225.991	-68.820	100.555	1.00	60.26	A
	ATOM O	2040	O	GLU A 379	224.963	-68.191	100.746	1.00	70.86	A
55	ATOM N	2041	N	HIS A 380	226.535	-69.606	101.468	1.00	54.34	A
	ATOM C	2042	CA	HIS A 380	225.921	-69.775	102.771	1.00	54.61	A
60	ATOM C	2043	CB	HIS A 380	226.975	-70.234	103.793	1.00	48.39	A
	ATOM C	2044	CG	HIS A 380	226.402	-70.617	105.121	1.00	45.24	A
	ATOM C	2045	CD2	HIS A 380	226.402	-71.793	105.781	1.00	42.14	A

	ATOM N	2046	ND1	HIS A	380	225.711	-69.731	105.921	1.00	51.46	A
	ATOM C	2047	CE1	HIS A	380	225.309	-70.349	107.018	1.00	50.88	A
5	ATOM N	2048	NE2	HIS A	380	225.715	-71.604	106.957	1.00	47.24	A
	ATOM C	2049	C	HIS A	380	225.231	-68.502	103.261	1.00	55.95	A
10	ATOM O	2050	O	HIS A	380	225.807	-67.409	103.206	1.00	60.83	A
	ATOM N	2051	N	PRO A	381	223.970	-68.630	103.727	1.00	55.60	A
	ATOM C	2052	CD	PRO A	381	223.229	-69.910	103.809	1.00	51.69	A
15	ATOM C	2053	CA	PRO A	381	223.147	-67.522	104.248	1.00	53.48	A
	ATOM C	2054	CB	PRO A	381	221.997	-68.257	104.936	1.00	49.53	A
20	ATOM C	2055	CG	PRO A	381	221.820	-69.442	104.035	1.00	49.24	A
	ATOM C	2056	C	PRO A	381	223.875	-66.545	105.212	1.00	56.98	A
	ATOM O	2057	O	PRO A	381	223.758	-65.320	105.074	1.00	59.03	A
25	ATOM N	2058	N	TRP A	382	224.635	-67.091	106.164	1.00	54.77	A
	ATOM C	2059	CA	TRP A	382	225.340	-66.282	107.146	1.00	55.06	A
30	ATOM C	2060	CB	TRP A	382	225.971	-67.165	108.240	1.00	54.64	A
	ATOM C	2061	CG	TRP A	382	226.691	-66.368	109.261	1.00	55.47	A
	ATOM C	2062	CD2	TRP A	382	228.111	-66.195	109.372	1.00	58.05	A
35	ATOM C	2063	CE2	TRP A	382	228.344	-65.342	110.476	1.00	60.80	A
	ATOM C	2064	CE3	TRP A	382	229.210	-66.680	108.649	1.00	60.95	A
40	ATOM C	2065	CD1	TRP A	382	226.137	-65.634	110.266	1.00	58.89	A
	ATOM N	2066	NE1	TRP A	382	227.123	-65.011	111.004	1.00	59.37	A
	ATOM C	2067	CZ2	TRP A	382	229.632	-64.965	110.871	1.00	64.01	A
45	ATOM C	2068	CZ3	TRP A	382	230.491	-66.302	109.042	1.00	60.80	A
	ATOM C	2069	CH2	TRP A	382	230.688	-65.458	110.140	1.00	65.05	A
50	ATOM C	2070	C	TRP A	382	226.397	-65.476	106.455	1.00	50.36	A
	ATOM O	2071	O	TRP A	382	226.579	-64.300	106.749	1.00	56.46	A
	ATOM N	2072	N	ILE A	383	227.094	-66.115	105.527	1.00	50.17	A
55	ATOM C	2073	CA	ILE A	383	228.163	-65.454	104.757	1.00	51.21	A
	ATOM C	2074	CB	ILE A	383	228.914	-66.460	103.856	1.00	42.86	A
60	ATOM C	2075	CG2	ILE A	383	229.642	-65.709	102.766	1.00	42.15	A
	ATOM C	2076	CG1	ILE A	383	229.846	-67.329	104.708	1.00	40.04	A

Residue	Atom	Seq. No.	Chain	Res. Name	X (Å)	Y (Å)	Z (Å)	Occup.	B-factor	Disorder
5	ATOM C	2077	CD1	ILE A 383	230.943	-66.520	105.429	1.00	40.46	A
	ATOM C	2078	C	ILE A 383	227.659	-64.305	103.873	1.00	52.36	A
	ATOM O	2079	O	ILE A 383	228.247	-63.229	103.858	1.00	51.23	A
	ATOM N	2080	N	THR A 384	226.553	-64.533	103.166	1.00	54.23	A
10	ATOM C	2081	CA	THR A 384	225.978	-63.535	102.275	1.00	58.09	A
	ATOM C	2082	CB	THR A 384	225.046	-64.197	101.265	1.00	57.25	A
15	ATOM O	2083	OG1	THR A 384	224.320	-65.235	101.920	1.00	65.44	A
	ATOM C	2084	CG2	THR A 384	225.809	-64.804	100.133	1.00	59.94	A
	ATOM C	2085	C	THR A 384	225.221	-62.436	102.988	1.00	57.62	A
20	ATOM O	2086	O	THR A 384	224.929	-61.395	102.420	1.00	61.64	A
	ATOM N	2087	N	ALA A 385	224.911	-62.655	104.249	1.00	60.34	A
25	ATOM C	2088	CA	ALA A 385	224.195	-61.658	105.030	1.00	57.14	A
	ATOM C	2089	CB	ALA A 385	223.197	-62.376	105.944	1.00	61.04	A
	ATOM C	2090	C	ALA A 385	225.112	-60.735	105.867	1.00	57.68	A
30	ATOM O	2091	O	ALA A 385	224.644	-59.765	106.467	1.00	56.76	A
	ATOM N	2092	N	ASN A 386	226.405	-61.038	105.919	1.00	57.22	A
35	ATOM C	2093	CA	ASN A 386	227.312	-60.217	106.705	1.00	59.50	A
	ATOM C	2094	CB	ASN A 386	227.751	-60.993	107.939	1.00	58.18	A
	ATOM C	2095	CG	ASN A 386	226.583	-61.313	108.874	1.00	60.78	A
40	ATOM O	2096	OD1	ASN A 386	226.026	-60.419	109.536	1.00	55.54	A
	ATOM N	2097	ND2	ASN A 386	226.201	-62.591	108.923	1.00	55.70	A
45	ATOM C	2098	C	ASN A 386	228.540	-59.733	105.965	1.00	55.04	A
	ATOM O	2099	O	ASN A 386	229.128	-58.723	106.336	1.00	58.67	A
	ATOM N	2100	N	SER A 387	228.903	-60.444	104.906	1.00	58.95	A
50	ATOM C	2101	CA	SER A 387	230.095	-60.110	104.132	1.00	63.83	A
	ATOM C	2102	CB	SER A 387	230.472	-61.278	103.220	1.00	55.03	A
55	ATOM O	2103	OG	SER A 387	231.719	-61.061	102.599	1.00	57.80	A
	ATOM C	2104	C	SER A 387	229.865	-58.867	103.278	1.00	64.86	A
	ATOM O	2105	O	SER A 387	228.745	-58.607	102.826	1.00	68.20	A
60	ATOM N	2106	N	SER A 388	230.916	-58.091	103.063	1.00	67.77	A
	ATOM C	2107	CA	SER A 388	230.786	-56.912	102.251	1.00	71.39	A

5	ATOM C	2108	CB	SER A 388	231.430	-55.722	102.969	1.00	71.24	A
	ATOM O	2109	OG	SER A 388	232.815	-55.916	103.141	1.00	79.50	A
	ATOM C	2110	C	SER A 388	231.403	-57.150	100.872	1.00	71.24	A
	ATOM O	2111	O	SER A 388	231.024	-56.501	99.909	1.00	76.22	A
10	ATOM N	2112	N	LYS A 389	232.336	-58.091	100.767	1.00	70.18	A
	ATOM C	2113	CA	LYS A 389	232.951	-58.347	99.475	1.00	67.46	A
15	ATOM C	2114	CB	LYS A 389	234.459	-58.686	99.667	1.00	49.89	A
	ATOM C	2115	C	LYS A 389	232.216	-59.459	98.688	1.00	68.81	A
	ATOM O	2116	O	LYS A 389	231.441	-60.236	99.337	1.00	76.61	A
20	ATOM O	2117	OXT	LYS A 389	232.453	-59.564	97.435	1.00	76.72	A
	ATOM P	2118	PB	ADP S 531	257.416	-68.553	107.649	1.00	34.84	S
25	ATOM O	2119	O1B	ADP S 531	258.545	-67.776	107.191	1.00	50.81	S
	ATOM O	2120	O2B	ADP S 531	257.209	-69.880	106.879	1.00	48.35	S
	ATOM O	2121	O3B	ADP S 531	257.422	-68.756	109.226	1.00	53.79	S
30	ATOM P	2122	PA	ADP S 531	256.077	-66.204	106.616	1.00	35.25	S
	ATOM O	2123	O1A	ADP S 531	256.842	-66.123	105.373	1.00	33.66	S
35	ATOM O	2124	O2A	ADP S 531	254.551	-65.860	106.461	1.00	54.13	S
	ATOM O	2125	O3A	ADP S 531	256.162	-67.643	107.261	1.00	62.78	S
	ATOM O	2126	O5*	ADP S 531	256.892	-65.243	107.657	1.00	48.32	S
40	ATOM C	2127	C5*	ADP S 531	256.442	-65.218	109.085	1.00	61.70	S
	ATOM C	2128	C4*	ADP S 531	255.856	-63.898	109.556	1.00	46.54	S
45	ATOM O	2129	O4*	ADP S 531	256.542	-62.868	108.818	1.00	44.98	S
	ATOM C	2130	C3*	ADP S 531	254.372	-63.620	109.292	1.00	37.55	S
	ATOM O	2131	O3*	ADP S 531	253.658	-64.161	110.347	1.00	46.23	S
50	ATOM C	2132	C2*	ADP S 531	254.337	-62.080	109.181	1.00	46.36	S
	ATOM O	2133	O2*	ADP S 531	254.148	-61.399	110.423	1.00	42.59	S
55	ATOM C	2134	C1*	ADP S 531	255.710	-61.716	108.597	1.00	43.16	S
	ATOM N	2135	N9	ADP S 531	255.666	-61.436	107.162	1.00	48.23	S
	ATOM C	2136	C8	ADP S 531	255.946	-62.302	106.136	1.00	47.43	S
60	ATOM N	2137	N7	ADP S 531	255.811	-61.734	104.897	1.00	42.83	S
	ATOM C	2138	C5	ADP S 531	255.418	-60.464	105.177	1.00	40.36	S

	Atom	ID	Res	Chain	Seq	X	Y	Z	Occ	B	Dis
5	ATOM C	2139	C6	ADP	S 531	255.122	-59.337	104.279	1.00	44.75	S
	ATOM N	2140	N6	ADP	S 531	255.151	-59.400	102.949	1.00	22.67	S
	ATOM N	2141	N1	ADP	S 531	254.762	-58.153	104.964	1.00	40.38	S
	ATOM C	2142	C2	ADP	S 531	254.725	-58.057	106.364	1.00	50.55	S
10	ATOM N	2143	N3	ADP	S 531	254.992	-59.070	107.188	1.00	51.07	S
	ATOM C	2144	C4	ADP	S 531	255.351	-60.245	106.574	1.00	46.49	S
15	ATOM MG	2145	MG	MG2	X 1	254.502	-68.175	108.413	1.00	47.20	X
	ATOM MG	2146	MG	MG2	X 2	255.864	-71.389	106.282	1.00	52.14	X
20	ATOM O	2147	OH2	WAT	W 1	264.531	-71.881	94.078	1.00	38.88	W
	ATOM O	2148	OH2	WAT	W 2	242.403	-78.272	113.237	1.00	54.89	W
	ATOM O	2149	OH2	WAT	W 3	232.705	-62.634	117.460	1.00	37.08	W
25	ATOM O	2150	OH2	WAT	W 4	251.977	-73.020	102.685	1.00	62.00	W
	ATOM O	2151	OH2	WAT	W 5	275.163	-72.604	97.774	1.00	53.95	W
	ATOM O	2152	OH2	WAT	W 6	232.526	-85.909	111.573	1.00	35.05	W
30	ATOM O	2153	OH2	WAT	W 7	259.170	-71.102	103.608	1.00	40.42	W
	ATOM O	2154	OH2	WAT	W 8	249.904	-55.205	99.315	1.00	26.87	W
	ATOM O	2155	OH2	WAT	W 9	229.701	-63.236	117.265	1.00	25.50	W

ATOM

5	ATOM C	1	CB	SER A 123	174.078	193.853	20.627	1.00	33.78	A
	ATOM O	2	OG	SER A 123	173.358	193.080	21.584	1.00	34.86	A
	ATOM C	3	C	SER A 123	173.331	195.751	21.954	1.00	32.28	A
	ATOM O	4	O	SER A 123	174.318	196.187	22.580	1.00	32.38	A
10	ATOM N	5	N	SER A 123	174.192	196.109	19.556	1.00	32.09	A
15	ATOM C	6	CA	SER A 123	173.449	195.246	20.532	1.00	33.80	A
	ATOM N	7	N	LYS A 124	172.107	195.682	22.463	1.00	30.56	A
	ATOM C	8	CA	LYS A 124	171.860	196.059	23.849	1.00	31.07	A
20	ATOM C	9	CB	LYS A 124	170.483	196.727	24.005	1.00	31.64	A
	ATOM C	10	CG	LYS A 124	170.231	197.847	23.021	1.00	33.77	A
	ATOM C	11	CD	LYS A 124	168.734	198.157	22.847	1.00	35.14	A
25	ATOM C	12	CE	LYS A 124	168.571	198.989	21.582	1.00	38.52	A
	ATOM N	13	NZ	LYS A 124	167.170	199.182	21.123	1.00	40.74	A
30	ATOM C	14	C	LYS A 124	171.929	194.785	24.714	1.00	30.29	A
	ATOM O	15	O	LYS A 124	171.724	194.845	25.913	1.00	30.99	A
	ATOM N	16	N	LYS A 125	172.256	193.646	24.102	1.00	30.71	A
35	ATOM C	17	CA	LYS A 125	172.352	192.375	24.835	1.00	29.50	A
	ATOM C	18	CB	LYS A 125	171.942	191.210	23.951	1.00	32.42	A
40	ATOM C	19	CG	LYS A 125	170.496	191.147	23.609	1.00	35.74	A
	ATOM C	20	CD	LYS A 125	170.221	189.915	22.777	1.00	38.96	A
	ATOM C	21	CE	LYS A 125	168.757	189.905	22.351	1.00	44.54	A
45	ATOM N	22	NZ	LYS A 125	168.305	188.576	21.807	1.00	44.21	A
	ATOM C	23	C	LYS A 125	173.728	192.027	25.381	1.00	26.48	A
50	ATOM O	24	O	LYS A 125	174.769	192.438	24.859	1.00	24.13	A
	ATOM N	25	N	ARG A 126	173.713	191.215	26.421	1.00	24.15	A
	ATOM C	26	CA	ARG A 126	174.952	190.756	27.020	1.00	22.33	A
55	ATOM C	27	CB	ARG A 126	174.636	189.835	28.191	1.00	21.13	A
	ATOM C	28	CG	ARG A 126	175.841	189.331	28.897	1.00	18.73	A
60	ATOM C	29	CD	ARG A 126	175.395	188.263	29.847	1.00	19.74	A
	ATOM N	30	NE	ARG A 126	176.552	187.628	30.420	1.00	16.73	A

5	ATOM C	31	CZ	ARG	A	126	176.503	186.741	31.394	1.00	17.59	A
	ATOM N	32	NH1	ARG	A	126	175.331	186.391	31.902	1.00	16.71	A
	ATOM N	33	NH2	ARG	A	126	177.633	186.214	31.854	1.00	18.45	A
	ATOM C	34	C	ARG	A	126	175.752	189.995	25.943	1.00	22.44	A
10	ATOM O	35	O	ARG	A	126	175.252	189.077	25.296	1.00	20.29	A
	ATOM N	36	N	GLN	A	127	176.997	190.406	25.763	1.00	21.10	A
15	ATOM C	37	CA	GLN	A	127	177.904	189.815	24.787	1.00	19.12	A
	ATOM C	38	CB	GLN	A	127	178.707	190.934	24.102	1.00	18.99	A
20	ATOM C	39	CG	GLN	A	127	177.842	191.925	23.355	1.00	15.64	A
	ATOM C	40	CD	GLN	A	127	177.154	191.297	22.162	1.00	17.04	A
	ATOM O	41	OE1	GLN	A	127	177.748	191.151	21.093	1.00	21.45	A
	ATOM N	42	NE2	GLN	A	127	175.902	190.912	22.339	1.00	20.66	A
25	ATOM C	43	C	GLN	A	127	178.861	188.861	25.496	1.00	17.70	A
	ATOM O	44	O	GLN	A	127	179.049	188.941	26.715	1.00	13.46	A
30	ATOM N	45	N	TRP	A	128	179.460	187.956	24.735	1.00	16.62	A
	ATOM C	46	CA	TRP	A	128	180.411	187.014	25.303	1.00	14.25	A
35	ATOM C	47	CB	TRP	A	128	180.890	186.029	24.237	1.00	13.22	A
	ATOM C	48	CG	TRP	A	128	179.858	185.060	23.779	1.00	9.34	A
	ATOM C	49	CD2	TRP	A	128	179.264	184.022	24.557	1.00	13.44	A
40	ATOM C	50	CE2	TRP	A	128	178.396	183.304	23.704	1.00	11.84	A
	ATOM C	51	CE3	TRP	A	128	179.389	183.618	25.899	1.00	15.05	A
45	ATOM C	52	CD1	TRP	A	128	179.338	184.945	22.529	1.00	11.79	A
	ATOM N	53	NE1	TRP	A	128	178.460	183.893	22.469	1.00	12.24	A
50	ATOM C	54	CZ2	TRP	A	128	177.648	182.204	24.146	1.00	10.99	A
	ATOM C	55	CZ3	TRP	A	128	178.646	182.523	26.336	1.00	15.81	A
	ATOM C	56	CH2	TRP	A	128	177.789	181.828	25.457	1.00	13.35	A
55	ATOM C	57	C	TRP	A	128	181.611	187.777	25.855	1.00	16.17	A
	ATOM O	58	O	TRP	A	128	181.885	188.903	25.457	1.00	17.48	A
60	ATOM N	59	N	ALA	A	129	182.306	187.146	26.790	1.00	17.52	A
	ATOM C	60	CA	ALA	A	129	183.501	187.695	27.415	1.00	17.26	A
	ATOM C	61	CB	ALA	A	129	183.129	188.595	28.576	1.00	8.15	A

	ATOM	62	C	ALA A 129	184.303	186.478	27.906	1.00	17.06	A
	C									
	ATOM	63	O	ALA A 129	183.733	185.426	28.198	1.00	17.77	A
	O									
5	ATOM	64	N	LEU A 130	185.618	186.620	27.979	1.00	16.79	A
	N									
	ATOM	65	CA	LEU A 130	186.479	185.540	28.425	1.00	19.53	A
	C									
10	ATOM	66	CB	LEU A 130	187.943	186.006	28.392	1.00	19.86	A
	C									
	ATOM	67	CG	LEU A 130	189.050	184.967	28.619	1.00	22.85	A
	C									
	ATOM	68	CD1	LEU A 130	188.897	183.839	27.604	1.00	17.77	A
	C									
15	ATOM	69	CD2	LEU A 130	190.429	185.631	28.492	1.00	16.04	A
	C									
	ATOM	70	C	LEU A 130	186.090	185.081	29.834	1.00	21.19	A
	C									
20	ATOM	71	O	LEU A 130	186.080	183.885	30.121	1.00	24.25	A
	O									
	ATOM	72	N	GLU A 131	185.756	186.032	30.705	1.00	23.78	A
	N									
	ATOM	73	CA	GLU A 131	185.349	185.729	32.082	1.00	25.83	A
	C									
25	ATOM	74	CB	GLU A 131	184.952	187.016	32.834	1.00	30.42	A
	C									
	ATOM	75	CG	GLU A 131	186.005	188.110	32.945	1.00	42.06	A
	C									
30	ATOM	76	CD	GLU A 131	186.135	188.977	31.686	1.00	46.89	A
	C									
	ATOM	77	OE1	GLU A 131	185.319	188.822	30.747	1.00	51.89	A
	O									
	ATOM	78	OE2	GLU A 131	187.058	189.821	31.640	1.00	50.51	A
	O									
35	ATOM	79	C	GLU A 131	184.146	184.751	32.145	1.00	25.30	A
	C									
	ATOM	80	O	GLU A 131	183.790	184.281	33.227	1.00	21.67	A
	O									
40	ATOM	81	N	ASP A 132	183.503	184.473	31.008	1.00	22.51	A
	N									
	ATOM	82	CA	ASP A 132	182.364	183.565	30.989	1.00	22.54	A
	C									
	ATOM	83	CB	ASP A 132	181.458	183.825	29.782	1.00	24.79	A
	C									
45	ATOM	84	CG	ASP A 132	180.631	185.120	29.908	1.00	28.99	A
	C									
	ATOM	85	OD1	ASP A 132	180.136	185.417	31.025	1.00	29.67	A
	O									
50	ATOM	86	OD2	ASP A 132	180.450	185.824	28.873	1.00	26.45	A
	O									
	ATOM	87	C	ASP A 132	182.752	182.087	30.966	1.00	21.99	A
	C									
	ATOM	88	O	ASP A 132	181.925	181.226	31.267	1.00	22.12	A
	O									
55	ATOM	89	N	PHE A 133	183.998	181.781	30.625	1.00	23.02	A
	N									
	ATOM	90	CA	PHE A 133	184.411	180.378	30.554	1.00	22.89	A
	C									
60	ATOM	91	CB	PHE A 133	184.812	179.998	29.111	1.00	18.64	A
	C									
	ATOM	92	CG	PHE A 133	183.901	180.565	28.039	1.00	17.41	A
	C									

5	ATOM C	93	CD1	PHE	A	133	184.042	181.884	27.616	1.00	15.80	A
	ATOM C	94	CD2	PHE	A	133	182.904	179.783	27.456	1.00	16.46	A
	ATOM C	95	CE1	PHE	A	133	183.215	182.414	26.637	1.00	14.66	A
	ATOM C	96	CE2	PHE	A	133	182.063	180.305	26.466	1.00	15.10	A
	ATOM C	97	CZ	PHE	A	133	182.224	181.626	26.060	1.00	18.42	A
10	ATOM C	98	C	PHE	A	133	185.557	179.984	31.484	1.00	22.91	A
	ATOM O	99	O	PHE	A	133	186.466	180.766	31.755	1.00	24.66	A
15	ATOM N	100	N	GLU	A	134	185.484	178.767	32.005	1.00	22.49	A
	ATOM C	101	CA	GLU	A	134	186.566	178.248	32.814	1.00	21.74	A
20	ATOM C	102	CB	GLU	A	134	186.054	177.264	33.870	1.00	23.93	A
	ATOM C	103	CG	GLU	A	134	185.401	177.912	35.088	1.00	29.62	A
25	ATOM C	104	CD	GLU	A	134	184.751	176.887	36.020	1.00	37.53	A
	ATOM O	105	OE1	GLU	A	134	185.460	175.983	36.533	1.00	38.84	A
	ATOM O	106	OE2	GLU	A	134	183.517	176.974	36.236	1.00	43.58	A
30	ATOM C	107	C	GLU	A	134	187.313	177.528	31.695	1.00	21.49	A
	ATOM O	108	O	GLU	A	134	186.702	176.784	30.922	1.00	23.43	A
35	ATOM N	109	N	ILE	A	135	188.608	177.794	31.564	1.00	19.74	A
	ATOM C	110	CA	ILE	A	135	189.425	177.197	30.524	1.00	19.08	A
	ATOM C	111	CB	ILE	A	135	190.554	178.149	30.072	1.00	22.58	A
40	ATOM C	112	CG2	ILE	A	135	191.285	177.543	28.866	1.00	19.44	A
	ATOM C	113	CG1	ILE	A	135	189.990	179.541	29.762	1.00	20.52	A
45	ATOM C	114	CD1	ILE	A	135	188.876	179.535	28.771	1.00	21.85	A
	ATOM C	115	C	ILE	A	135	190.099	175.941	31.044	1.00	20.74	A
	ATOM O	116	O	ILE	A	135	190.667	175.944	32.140	1.00	19.34	A
50	ATOM N	117	N	GLY	A	136	190.058	174.876	30.245	1.00	19.98	A
	ATOM C	118	CA	GLY	A	136	190.688	173.629	30.637	1.00	19.38	A
55	ATOM C	119	C	GLY	A	136	191.995	173.397	29.906	1.00	18.61	A
	ATOM O	120	O	GLY	A	136	192.742	174.324	29.668	1.00	20.61	A
60	ATOM N	121	N	ARG	A	137	192.267	172.156	29.533	1.00	22.50	A
	ATOM C	122	CA	ARG	A	137	193.500	171.827	28.833	1.00	22.75	A
	ATOM C	123	CB	ARG	A	137	193.771	170.325	28.920	1.00	22.49	A

	ATOM C	124	CG	ARG A	137	192.820	169.474	28.047	1.00	20.82	A
	ATOM C	125	CD	ARG A	137	193.107	168.016	28.252	1.00	15.70	A
5	ATOM N	126	NE	ARG A	137	192.212	167.104	27.554	1.00	14.70	A
	ATOM C	127	CZ	ARG A	137	192.299	166.784	26.266	1.00	14.90	A
10	ATOM N	128	NH1	ARG A	137	193.237	167.305	25.493	1.00	13.75	A
	ATOM N	129	NH2	ARG A	137	191.462	165.900	25.758	1.00	13.41	A
	ATOM C	130	C	ARG A	137	193.396	172.183	27.357	1.00	23.53	A
15	ATOM O	131	O	ARG A	137	192.316	172.425	26.840	1.00	24.10	A
	ATOM N	132	N	PRO A	138	194.542	172.250	26.671	1.00	22.98	A
20	ATOM C	133	CD	PRO A	138	195.850	172.477	27.313	1.00	19.97	A
	ATOM C	134	CA	PRO A	138	194.613	172.552	25.237	1.00	22.67	A
	ATOM C	135	CB	PRO A	138	196.116	172.791	25.007	1.00	21.39	A
25	ATOM C	136	CG	PRO A	138	196.570	173.354	26.295	1.00	19.67	A
	ATOM C	137	C	PRO A	138	194.135	171.275	24.497	1.00	23.48	A
30	ATOM O	138	O	PRO A	138	194.528	170.147	24.876	1.00	21.67	A
	ATOM N	139	N	LEU A	139	193.297	171.435	23.471	1.00	19.70	A
	ATOM C	140	CA	LEU A	139	192.809	170.281	22.716	1.00	19.33	A
35	ATOM C	141	CB	LEU A	139	191.340	170.454	22.318	1.00	19.32	A
	ATOM C	142	CG	LEU A	139	190.349	170.509	23.473	1.00	18.46	A
40	ATOM C	143	CD1	LEU A	139	188.966	170.866	22.964	1.00	16.26	A
	ATOM C	144	CD2	LEU A	139	190.342	169.178	24.163	1.00	15.61	A
	ATOM C	145	C	LEU A	139	193.636	170.125	21.454	1.00	18.97	A
45	ATOM O	146	O	LEU A	139	193.714	169.045	20.883	1.00	20.68	A
	ATOM N	147	N	GLY A	140	194.256	171.215	21.026	1.00	19.57	A
50	ATOM C	148	CA	GLY A	140	195.056	171.181	19.825	1.00	16.45	A
	ATOM C	149	C	GLY A	140	195.821	172.461	19.630	1.00	18.41	A
	ATOM O	150	O	GLY A	140	195.560	173.469	20.280	1.00	17.66	A
55	ATOM N	151	N	LYS A	141	196.778	172.413	18.713	1.00	23.54	A
	ATOM C	152	CA	LYS A	141	197.635	173.547	18.399	1.00	25.64	A
60	ATOM C	153	CB	LYS A	141	199.103	173.104	18.473	1.00	29.50	A
	ATOM C	154	CG	LYS A	141	200.101	174.192	18.080	1.00	37.58	A

5	ATOM C	155	CD	LYS A 141	201.550	173.744	18.187	1.00	42.29	A
	ATOM C	156	CE	LYS A 141	202.483	174.918	17.891	1.00	46.12	A
	ATOM N	157	NZ	LYS A 141	203.914	174.481	17.890	1.00	49.84	A
	ATOM C	158	C	LYS A 141	197.313	174.071	16.995	1.00	26.94	A
10	ATOM O	159	O	LYS A 141	197.578	173.409	15.986	1.00	26.47	A
	ATOM N	160	N	GLY A 142	196.724	175.256	16.938	1.00	26.51	A
15	ATOM C	161	CA	GLY A 142	196.392	175.839	15.656	1.00	26.65	A
	ATOM C	162	C	GLY A 142	197.515	176.753	15.234	1.00	26.71	A
	ATOM O	163	O	GLY A 142	198.384	177.086	16.052	1.00	26.93	A
20	ATOM N	164	N	LYS A 143	197.501	177.158	13.969	1.00	24.67	A
	ATOM C	165	CA	LYS A 143	198.529	178.037	13.452	1.00	22.25	A
25	ATOM C	166	CB	LYS A 143	198.362	178.220	11.925	1.00	25.89	A
	ATOM C	167	CG	LYS A 143	199.535	178.982	11.307	1.00	30.09	A
	ATOM C	168	CD	LYS A 143	199.516	179.060	9.792	1.00	35.88	A
30	ATOM C	169	CE	LYS A 143	200.619	180.037	9.330	1.00	41.66	A
	ATOM N	170	NZ	LYS A 143	200.871	180.206	7.857	1.00	42.97	A
35	ATOM C	171	C	LYS A 143	198.554	179.404	14.160	1.00	22.22	A
	ATOM O	172	O	LYS A 143	199.641	179.921	14.425	1.00	22.44	A
	ATOM N	173	N	PHE A 144	197.394	179.986	14.477	1.00	20.35	A
40	ATOM C	174	CA	PHE A 144	197.370	181.311	15.130	1.00	21.42	A
	ATOM C	175	CB	PHE A 144	196.429	182.258	14.362	1.00	17.68	A
45	ATOM C	176	CG	PHE A 144	196.798	182.429	12.896	1.00	22.16	A
	ATOM C	177	CD1	PHE A 144	196.541	181.421	11.959	1.00	20.33	A
	ATOM C	178	CD2	PHE A 144	197.460	183.574	12.464	1.00	23.47	A
50	ATOM C	179	CE1	PHE A 144	196.944	181.564	10.624	1.00	20.91	A
	ATOM C	180	CE2	PHE A 144	197.864	183.716	11.128	1.00	21.10	A
55	ATOM C	181	CZ	PHE A 144	197.606	182.708	10.213	1.00	18.55	A
	ATOM C	182	C	PHE A 144	197.001	181.263	16.626	1.00	20.47	A
	ATOM O	183	O	PHE A 144	196.668	182.283	17.246	1.00	20.98	A
60	ATOM N	184	N	GLY A 145	197.094	180.072	17.208	1.00	18.58	A
	ATOM C	185	CA	GLY A 145	196.786	179.915	18.616	1.00	19.23	A

5	ATOM C	186	C	GLY	A	145	196.229	178.538	18.922	1.00	20.99	A
	ATOM O	187	O	GLY	A	145	195.911	177.756	18.016	1.00	21.28	A
	ATOM N	188	N	ASN	A	146	196.100	178.233	20.204	1.00	20.66	A
	ATOM C	189	CA	ASN	A	146	195.574	176.938	20.598	1.00	21.26	A
10	ATOM C	190	CB	ASN	A	146	196.140	176.544	21.964	1.00	24.59	A
	ATOM C	191	CG	ASN	A	146	197.638	176.352	21.939	1.00	27.16	A
15	ATOM O	192	OD1	ASN	A	146	198.205	175.853	20.956	1.00	32.36	A
	ATOM N	193	ND2	ASN	A	146	198.292	176.737	23.015	1.00	27.51	A
	ATOM C	194	C	ASN	A	146	194.056	176.878	20.683	1.00	20.53	A
20	ATOM O	195	O	ASN	A	146	193.370	177.902	20.676	1.00	20.90	A
	ATOM N	196	N	VAL	A	147	193.540	175.658	20.740	1.00	18.03	A
25	ATOM C	197	CA	VAL	A	147	192.121	175.430	20.922	1.00	14.64	A
	ATOM C	198	CB	VAL	A	147	191.528	174.515	19.799	1.00	13.96	A
	ATOM C	199	CG1	VAL	A	147	190.053	174.217	20.092	1.00	10.05	A
30	ATOM C	200	CG2	VAL	A	147	191.669	175.213	18.439	1.00	8.41	A
	ATOM C	201	C	VAL	A	147	192.142	174.746	22.301	1.00	16.21	A
35	ATOM O	202	O	VAL	A	147	192.897	173.783	22.523	1.00	14.13	A
	ATOM N	203	N	TYR	A	148	191.375	175.299	23.242	1.00	14.89	A
	ATOM C	204	CA	TYR	A	148	191.315	174.786	24.614	1.00	14.47	A
40	ATOM C	205	CB	TYR	A	148	191.593	175.891	25.642	1.00	12.68	A
	ATOM C	206	CG	TYR	A	148	192.910	176.619	25.491	1.00	18.66	A
45	ATOM C	207	CD1	TYR	A	148	193.031	177.690	24.605	1.00	16.46	A
	ATOM C	208	CE1	TYR	A	148	194.243	178.347	24.434	1.00	18.77	A
	ATOM C	209	CD2	TYR	A	148	194.047	176.222	26.217	1.00	15.67	A
50	ATOM C	210	CE2	TYR	A	148	195.269	176.880	26.050	1.00	20.14	A
	ATOM C	211	CZ	TYR	A	148	195.355	177.938	25.153	1.00	18.86	A
55	ATOM O	212	OH	TYR	A	148	196.555	178.569	24.934	1.00	23.63	A
	ATOM C	213	C	TYR	A	148	189.943	174.234	24.936	1.00	13.13	A
	ATOM O	214	O	TYR	A	148	188.942	174.674	24.386	1.00	14.07	A
60	ATOM N	215	N	LEU	A	149	189.887	173.265	25.831	1.00	11.62	A
	ATOM C	216	CA	LEU	A	149	188.600	172.753	26.223	1.00	11.86	A

5	ATOM C	217	CB	LEU A 149	188.787	171.466	27.003	1.00	10.50	A
	ATOM C	218	CG	LEU A 149	187.547	170.675	27.388	1.00	12.61	A
	ATOM C	219	CD1	LEU A 149	186.695	170.364	26.182	1.00	11.20	A
	ATOM C	220	CD2	LEU A 149	188.001	169.410	28.051	1.00	11.24	A
10	ATOM C	221	C	LEU A 149	188.071	173.911	27.101	1.00	13.55	A
	ATOM O	222	O	LEU A 149	188.857	174.728	27.565	1.00	12.48	A
15	ATOM N	223	N	ALA A 150	186.763	174.008	27.316	1.00	14.24	A
	ATOM C	224	CA	ALA A 150	186.227	175.102	28.120	1.00	15.20	A
20	ATOM C	225	CB	ALA A 150	186.230	176.406	27.318	1.00	15.60	A
	ATOM C	226	C	ALA A 150	184.817	174.800	28.612	1.00	17.25	A
	ATOM O	227	O	ALA A 150	184.122	173.929	28.083	1.00	18.30	A
	ATOM N	228	N	ARG A 151	184.398	175.532	29.629	1.00	17.29	A
25	ATOM C	229	CA	ARG A 151	183.091	175.334	30.215	1.00	19.70	A
	ATOM C	230	CB	ARG A 151	183.245	174.479	31.492	1.00	20.02	A
30	ATOM C	231	CG	ARG A 151	181.977	174.102	32.258	1.00	26.58	A
	ATOM C	232	CD	ARG A 151	182.321	173.557	33.686	1.00	30.64	A
35	ATOM N	233	NE	ARG A 151	183.235	172.405	33.673	1.00	32.15	A
	ATOM C	234	CZ	ARG A 151	182.900	171.151	33.348	1.00	33.18	A
	ATOM N	235	NH1	ARG A 151	181.644	170.851	33.004	1.00	33.09	A
40	ATOM N	236	NH2	ARG A 151	183.831	170.190	33.362	1.00	31.48	A
	ATOM C	237	C	ARG A 151	182.516	176.707	30.518	1.00	20.61	A
45	ATOM O	238	O	ARG A 151	183.158	177.560	31.163	1.00	19.62	A
	ATOM N	239	N	GLU A 152	181.315	176.939	30.006	1.00	21.84	A
50	ATOM C	240	CA	GLU A 152	180.633	178.196	30.264	1.00	21.85	A
	ATOM C	241	CB	GLU A 152	179.401	178.298	29.377	1.00	26.06	A
	ATOM C	242	CG	GLU A 152	178.766	179.690	29.289	1.00	28.31	A
	ATOM C	243	CD	GLU A 152	177.996	180.078	30.543	1.00	32.60	A
55	ATOM O	244	OE1	GLU A 152	178.576	180.804	31.391	1.00	33.50	A
	ATOM O	245	OE2	GLU A 152	176.821	179.650	30.679	1.00	29.24	A
60	ATOM C	246	C	GLU A 152	180.252	178.091	31.742	1.00	21.10	A
	ATOM O	247	O	GLU A 152	179.661	177.102	32.172	1.00	19.62	A

5	ATOM N	248	N	LYS A 153	180.613	179.114	32.504	1.00	21.06	A
	ATOM C	249	CA	LYS A 153	180.366	179.156	33.933	1.00	20.90	A
	ATOM C	250	CB	LYS A 153	180.996	180.417	34.513	1.00	20.37	A
	ATOM C	251	CG	LYS A 153	182.501	180.458	34.440	1.00	22.17	A
10	ATOM C	252	CD	LYS A 153	183.063	181.720	35.091	1.00	21.22	A
	ATOM C	253	CE	LYS A 153	184.568	181.658	35.002	1.00	22.77	A
15	ATOM N	254	NZ	LYS A 153	185.178	182.877	35.572	1.00	24.11	A
	ATOM C	255	C	LYS A 153	178.927	179.048	34.421	1.00	21.26	A
	ATOM O	256	O	LYS A 153	178.649	178.362	35.390	1.00	25.58	A
20	ATOM N	257	N	GLN A 154	177.982	179.704	33.786	1.00	23.03	A
	ATOM C	258	CA	GLN A 154	176.639	179.579	34.330	1.00	23.96	A
25	ATOM C	259	CB	GLN A 154	175.744	180.686	33.800	1.00	23.79	A
	ATOM C	260	CG	GLN A 154	176.125	182.053	34.288	1.00	24.55	A
	ATOM C	261	CD	GLN A 154	175.243	183.133	33.709	1.00	24.55	A
30	ATOM O	262	OE1	GLN A 154	175.674	184.283	33.617	1.00	23.87	A
	ATOM N	263	NE2	GLN A 154	173.998	182.779	33.309	1.00	22.50	A
35	ATOM C	264	C	GLN A 154	175.951	178.229	34.086	1.00	24.10	A
	ATOM O	265	O	GLN A 154	175.345	177.675	34.996	1.00	25.34	A
	ATOM N	266	N	SER A 155	176.018	177.700	32.871	1.00	22.36	A
40	ATOM C	267	CA	SER A 155	175.351	176.441	32.585	1.00	21.24	A
	ATOM C	268	CB	SER A 155	174.790	176.517	31.180	1.00	20.38	A
45	ATOM O	269	OG	SER A 155	175.875	176.607	30.282	1.00	22.24	A
	ATOM C	270	C	SER A 155	176.234	175.182	32.691	1.00	23.66	A
	ATOM O	271	O	SER A 155	175.725	174.048	32.677	1.00	20.04	A
50	ATOM N	272	N	LYS A 156	177.549	175.406	32.789	1.00	23.61	A
	ATOM C	273	CA	LYS A 156	178.572	174.358	32.849	1.00	24.47	A
55	ATOM C	274	CB	LYS A 156	178.350	173.467	34.065	1.00	25.24	A
	ATOM C	275	CG	LYS A 156	178.523	174.254	35.368	1.00	32.64	A
	ATOM C	276	CD	LYS A 156	178.309	173.358	36.552	1.00	35.73	A
60	ATOM C	277	CE	LYS A 156	178.506	174.079	37.870	1.00	41.50	A
	ATOM N	278	NZ	LYS A 156	178.457	173.059	38.978	1.00	42.75	A

5	ATOM C	279	C	LYS A 156	178.634	173.543	31.548	1.00	22.03	A
	ATOM O	280	O	LYS A 156	179.131	172.417	31.509	1.00	22.31	A
	ATOM N	281	N	PHE A 157	178.152	174.152	30.472	1.00	20.94	A
	ATOM C	282	CA	PHE A 157	178.180	173.530	29.162	1.00	19.88	A
	ATOM C	283	CB	PHE A 157	177.370	174.367	28.174	1.00	21.87	A
10	ATOM C	284	CG	PHE A 157	177.209	173.735	26.840	1.00	22.62	A
	ATOM C	285	CD1	PHE A 157	176.501	172.546	26.704	1.00	26.84	A
15	ATOM C	286	CD2	PHE A 157	177.745	174.336	25.707	1.00	24.18	A
	ATOM C	287	CE1	PHE A 157	176.326	171.957	25.448	1.00	27.13	A
	ATOM C	288	CE2	PHE A 157	177.576	173.763	24.446	1.00	24.84	A
20	ATOM C	289	CZ	PHE A 157	176.868	172.574	24.316	1.00	26.19	A
	ATOM C	290	C	PHE A 157	179.645	173.447	28.708	1.00	20.86	A
25	ATOM O	291	O	PHE A 157	180.394	174.451	28.739	1.00	16.68	A
	ATOM N	292	N	ILE A 158	180.056	172.243	28.316	1.00	18.62	A
30	ATOM C	293	CA	ILE A 158	181.412	171.997	27.862	1.00	17.65	A
	ATOM C	294	CB	ILE A 158	181.818	170.521	28.156	1.00	21.22	A
	ATOM C	295	CG2	ILE A 158	183.120	170.183	27.472	1.00	20.54	A
35	ATOM C	296	CG1	ILE A 158	181.998	170.339	29.675	1.00	25.44	A
	ATOM C	297	CD1	ILE A 158	181.751	168.898	30.193	1.00	32.22	A
40	ATOM C	298	C	ILE A 158	181.502	172.306	26.363	1.00	19.32	A
	ATOM O	299	O	ILE A 158	180.622	171.940	25.588	1.00	21.25	A
45	ATOM N	300	N	LEU A 159	182.544	173.021	25.958	1.00	19.68	A
	ATOM C	301	CA	LEU A 159	182.729	173.365	24.552	1.00	18.03	A
	ATOM C	302	CB	LEU A 159	181.915	174.625	24.214	1.00	18.70	A
50	ATOM C	303	CG	LEU A 159	181.855	175.726	25.275	1.00	18.81	A
	ATOM C	304	CD1	LEU A 159	183.137	176.522	25.197	1.00	25.89	A
55	ATOM C	305	CD2	LEU A 159	180.667	176.644	25.065	1.00	15.33	A
	ATOM C	306	C	LEU A 159	184.218	173.553	24.263	1.00	16.64	A
	ATOM O	307	O	LEU A 159	185.054	173.211	25.099	1.00	10.64	A
60	ATOM N	308	N	ALA A 160	184.562	174.069	23.084	1.00	14.09	A
	ATOM C	309	CA	ALA A 160	185.981	174.271	22.742	1.00	14.90	A

	Atom	ID	Type	Label	Res	B-factor	Occupancy	Q-score	R-factor	R-free	Weight
5	ATOM C	310	CB	ALA A	160	186.371	173.394	21.574	1.00	11.94	A
	ATOM C	311	C	ALA A	160	186.230	175.736	22.420	1.00	15.35	A
	ATOM O	312	O	ALA A	160	185.419	176.377	21.777	1.00	16.22	A
	ATOM N	313	N	LEU A	161	187.348	176.277	22.876	1.00	17.51	A
10	ATOM C	314	CA	LEU A	161	187.656	177.685	22.636	1.00	17.81	A
	ATOM C	315	CB	LEU A	161	187.959	178.379	23.958	1.00	19.09	A
	ATOM C	316	CG	LEU A	161	187.661	179.882	24.003	1.00	24.28	A
15	ATOM C	317	CD1	LEU A	161	186.190	180.085	23.715	1.00	19.74	A
	ATOM C	318	CD2	LEU A	161	188.020	180.482	25.396	1.00	26.64	A
20	ATOM C	319	C	LEU A	161	188.857	177.829	21.697	1.00	18.94	A
	ATOM O	320	O	LEU A	161	189.984	177.506	22.070	1.00	15.15	A
25	ATOM N	321	N	LYS A	162	188.605	178.302	20.477	1.00	15.44	A
	ATOM C	322	CA	LYS A	162	189.671	178.489	19.506	1.00	16.27	A
30	ATOM C	323	CB	LYS A	162	189.142	178.254	18.093	1.00	15.06	A
	ATOM C	324	CG	LYS A	162	190.184	178.338	17.036	1.00	13.12	A
	ATOM C	325	CD	LYS A	162	189.615	177.968	15.682	1.00	15.23	A
35	ATOM C	326	CE	LYS A	162	190.694	178.025	14.590	1.00	15.94	A
	ATOM N	327	NZ	LYS A	162	190.118	177.625	13.262	1.00	21.75	A
	ATOM C	328	C	LYS A	162	190.220	179.909	19.626	1.00	16.04	A
40	ATOM O	329	O	LYS A	162	189.486	180.863	19.427	1.00	17.16	A
	ATOM N	330	N	VAL A	163	191.501	180.044	19.955	1.00	15.21	A
45	ATOM C	331	CA	VAL A	163	192.110	181.357	20.107	1.00	16.50	A
	ATOM C	332	CB	VAL A	163	193.047	181.400	21.336	1.00	17.79	A
	ATOM C	333	CG1	VAL A	163	193.563	182.816	21.546	1.00	15.20	A
50	ATOM C	334	CG2	VAL A	163	192.316	180.897	22.578	1.00	14.92	A
	ATOM C	335	C	VAL A	163	192.938	181.758	18.888	1.00	17.82	A
55	ATOM O	336	O	VAL A	163	193.616	180.933	18.287	1.00	20.09	A
	ATOM N	337	N	LEU A	164	192.888	183.028	18.522	1.00	18.13	A
60	ATOM C	338	CA	LEU A	164	193.670	183.509	17.387	1.00	15.87	A
	ATOM C	339	CB	LEU A	164	192.747	183.802	16.203	1.00	18.86	A
	ATOM C	340	CG	LEU A	164	191.903	182.603	15.752	1.00	20.75	A

	ATOM C	341	CD1	LEU A 164	190.429	182.980	15.575	1.00	23.26	A
	ATOM C	342	CD2	LEU A 164	192.481	182.084	14.477	1.00	19.09	A
5	ATOM C	343	C	LEU A 164	194.352	184.789	17.835	1.00	16.04	A
	ATOM O	344	O	LEU A 164	193.687	185.709	18.295	1.00	13.41	A
10	ATOM N	345	N	PHE A 165	195.670	184.858	17.738	1.00	15.52	A
	ATOM C	346	CA	PHE A 165	196.340	186.082	18.141	1.00	18.33	A
	ATOM C	347	CB	PHE A 165	197.804	185.823	18.497	1.00	19.71	A
15	ATOM C	348	CG	PHE A 165	197.987	185.214	19.850	1.00	26.23	A
	ATOM C	349	CD1	PHE A 165	197.826	183.840	20.033	1.00	27.06	A
20	ATOM C	350	CD2	PHE A 165	198.222	186.025	20.961	1.00	28.47	A
	ATOM C	351	CE1	PHE A 165	197.899	183.281	21.298	1.00	32.07	A
	ATOM C	352	CE2	PHE A 165	198.299	185.479	22.239	1.00	31.56	A
25	ATOM C	353	CZ	PHE A 165	198.133	184.104	22.411	1.00	35.02	A
	ATOM C	354	C	PHE A 165	196.228	187.062	16.989	1.00	19.49	A
30	ATOM O	355	O	PHE A 165	196.610	186.742	15.857	1.00	21.60	A
	ATOM N	356	N	LYS A 166	195.674	188.242	17.277	1.00	18.17	A
	ATOM C	357	CA	LYS A 166	195.458	189.299	16.282	1.00	17.63	A
35	ATOM C	358	CB	LYS A 166	194.786	190.520	16.931	1.00	16.68	A
	ATOM C	359	CG	LYS A 166	193.319	190.346	17.376	1.00	15.54	A
40	ATOM C	360	CD	LYS A 166	192.703	191.672	17.826	1.00	10.39	A
	ATOM C	361	CE	LYS A 166	191.259	191.452	18.272	1.00	12.43	A
	ATOM N	362	NZ	LYS A 166	190.505	192.644	18.792	1.00	7.46	A
45	ATOM C	363	C	LYS A 166	196.696	189.792	15.536	1.00	19.44	A
	ATOM O	364	O	LYS A 166	196.615	190.103	14.343	1.00	19.53	A
50	ATOM N	365	N	ALA A 167	197.828	189.885	16.237	1.00	19.10	A
	ATOM C	366	CA	ALA A 167	199.068	190.369	15.628	1.00	18.82	A
	ATOM C	367	CB	ALA A 167	200.140	190.591	16.710	1.00	11.48	A
55	ATOM C	368	C	ALA A 167	199.551	189.377	14.571	1.00	18.71	A
	ATOM O	369	O	ALA A 167	200.085	189.762	13.534	1.00	19.61	A
60	ATOM N	370	N	GLN A 168	199.351	188.092	14.840	1.00	18.71	A
	ATOM C	371	CA	GLN A 168	199.734	187.039	13.907	1.00	18.86	A

5	ATOM C	372	CB	GLN A 168	199.584	185.666	14.561	1.00	21.65	A
	ATOM C	373	CG	GLN A 168	200.584	184.664	14.014	1.00	25.64	A
	ATOM C	374	CD	GLN A 168	200.544	183.310	14.690	1.00	29.19	A
	ATOM O	375	OE1	GLN A 168	200.269	183.208	15.900	1.00	27.17	A
10	ATOM N	376	NE2	GLN A 168	200.846	182.249	13.920	1.00	28.74	A
	ATOM C	377	C	GLN A 168	198.824	187.137	12.688	1.00	17.82	A
15	ATOM O	378	O	GLN A 168	199.273	187.079	11.560	1.00	20.56	A
	ATOM N	379	N	LEU A 169	197.530	187.289	12.931	1.00	19.46	A
20	ATOM C	380	CA	LEU A 169	196.553	187.404	11.848	1.00	19.86	A
	ATOM C	381	CB	LEU A 169	195.146	187.572	12.393	1.00	20.65	A
	ATOM C	382	CG	LEU A 169	194.514	186.370	13.052	1.00	24.58	A
25	ATOM C	383	CD1	LEU A 169	193.168	186.837	13.566	1.00	23.53	A
	ATOM C	384	CD2	LEU A 169	194.396	185.189	12.069	1.00	20.67	A
30	ATOM C	385	C	LEU A 169	196.802	188.604	10.961	1.00	21.12	A
	ATOM O	386	O	LEU A 169	196.533	188.564	9.761	1.00	17.39	A
	ATOM N	387	N	GLU A 170	197.261	189.697	11.564	1.00	22.51	A
35	ATOM C	388	CA	GLU A 170	197.520	190.915	10.807	1.00	23.02	A
	ATOM C	389	CB	GLU A 170	197.637	192.102	11.769	1.00	22.68	A
40	ATOM C	390	CG	GLU A 170	196.267	192.607	12.232	1.00	27.99	A
	ATOM C	391	CD	GLU A 170	196.294	193.330	13.579	1.00	31.84	A
	ATOM O	392	OE1	GLU A 170	197.334	193.955	13.920	1.00	33.33	A
45	ATOM O	393	OE2	GLU A 170	195.256	193.278	14.285	1.00	31.22	A
	ATOM C	394	C	GLU A 170	198.762	190.753	9.949	1.00	21.03	A
50	ATOM O	395	O	GLU A 170	198.739	191.068	8.757	1.00	23.09	A
	ATOM N	396	N	LYS A 171	199.826	190.220	10.535	1.00	17.25	A
	ATOM C	397	CA	LYS A 171	201.059	190.014	9.790	1.00	19.63	A
55	ATOM C	398	CB	LYS A 171	202.139	189.442	10.706	1.00	21.18	A
	ATOM C	399	CG	LYS A 171	203.525	189.395	10.073	1.00	25.15	A
60	ATOM C	400	CD	LYS A 171	204.574	188.888	11.054	1.00	28.24	A
	ATOM C	401	CE	LYS A 171	205.952	188.807	10.395	1.00	32.60	A
	ATOM N	402	NZ	LYS A 171	207.003	188.297	11.331	1.00	33.23	A

5	ATOM C	403	C	LYS A 171	200.838	189.074	8.609	1.00	19.42	A
	ATOM O	404	O	LYS A 171	201.451	189.235	7.551	1.00	21.92	A
	ATOM N	405	N	ALA A 172	199.957	188.095	8.782	1.00	17.92	A
	ATOM C	406	CA	ALA A 172	199.666	187.126	7.720	1.00	18.61	A
	ATOM C	407	CB	ALA A 172	199.168	185.826	8.341	1.00	13.39	A
10	ATOM C	408	C	ALA A 172	198.666	187.627	6.679	1.00	16.48	A
	ATOM O	409	O	ALA A 172	198.600	187.082	5.577	1.00	18.45	A
15	ATOM N	410	N	GLY A 173	197.890	188.651	7.053	1.00	16.48	A
	ATOM C	411	CA	GLY A 173	196.876	189.241	6.178	1.00	17.37	A
20	ATOM C	412	C	GLY A 173	195.719	188.297	5.904	1.00	18.48	A
	ATOM O	413	O	GLY A 173	195.158	188.264	4.789	1.00	17.50	A
25	ATOM N	414	N	VAL A 174	195.344	187.536	6.921	1.00	16.39	A
	ATOM C	415	CA	VAL A 174	194.274	186.573	6.770	1.00	18.80	A
30	ATOM C	416	CB	VAL A 174	194.778	185.171	7.226	1.00	17.75	A
	ATOM C	417	CG1	VAL A 174	195.976	184.770	6.371	1.00	17.03	A
35	ATOM C	418	CG2	VAL A 174	195.166	185.207	8.684	1.00	12.69	A
	ATOM C	419	C	VAL A 174	193.015	186.982	7.535	1.00	19.69	A
40	ATOM O	420	O	VAL A 174	192.152	186.152	7.828	1.00	22.14	A
	ATOM N	421	N	GLU A 175	192.900	188.282	7.801	1.00	24.29	A
45	ATOM C	422	CA	GLU A 175	191.751	188.834	8.521	1.00	25.76	A
	ATOM C	423	CB	GLU A 175	191.902	190.351	8.799	1.00	29.22	A
50	ATOM C	424	CG	GLU A 175	193.333	190.938	8.903	1.00	38.41	A
	ATOM O	425	CD	GLU A 175	193.998	191.112	7.548	1.00	39.97	A
55	ATOM O	426	OE1	GLU A 175	193.310	190.986	6.511	1.00	47.49	A
	ATOM O	427	OE2	GLU A 175	195.206	191.382	7.507	1.00	46.22	A
60	ATOM C	428	C	GLU A 175	190.452	188.611	7.752	1.00	25.95	A
	ATOM O	429	O	GLU A 175	189.423	188.313	8.337	1.00	25.42	A
65	ATOM N	430	N	HIS A 176	190.483	188.768	6.438	1.00	26.45	A
	ATOM C	431	CA	HIS A 176	189.254	188.539	5.708	1.00	24.68	A
70	ATOM C	432	CB	HIS A 176	189.316	189.074	4.278	1.00	23.09	A
	ATOM C	433	CG	HIS A 176	187.983	189.014	3.596	1.00	32.41	A

5	ATOM C	434	CD2	HIS	A	176	187.570	188.363	2.477	1.00	34.18	A
	ATOM N	435	ND1	HIS	A	176	186.845	189.576	4.148	1.00	32.75	A
	ATOM C	436	CE1	HIS	A	176	185.796	189.266	3.406	1.00	33.74	A
	ATOM N	437	NE2	HIS	A	176	186.207	188.529	2.386	1.00	34.72	A
10	ATOM C	438	C	HIS	A	176	188.848	187.062	5.703	1.00	23.32	A
	ATOM O	439	O	HIS	A	176	187.661	186.755	5.693	1.00	22.64	A
15	ATOM N	440	N	GLN	A	177	189.803	186.137	5.744	1.00	21.78	A
	ATOM C	441	CA	GLN	A	177	189.432	184.721	5.774	1.00	19.85	A
20	ATOM C	442	CB	GLN	A	177	190.628	183.818	5.421	1.00	21.23	A
	ATOM C	443	CG	GLN	A	177	191.173	183.994	3.977	1.00	23.08	A
	ATOM C	444	CD	GLN	A	177	192.113	185.179	3.856	1.00	26.14	A
	ATOM O	445	OE1	GLN	A	177	191.901	186.204	4.512	1.00	27.02	A
25	ATOM N	446	NE2	GLN	A	177	193.161	185.056	3.012	1.00	25.09	A
	ATOM C	447	C	GLN	A	177	188.859	184.317	7.129	1.00	18.66	A
30	ATOM O	448	O	GLN	A	177	188.057	183.390	7.195	1.00	18.16	A
	ATOM N	449	N	LEU	A	178	189.267	185.001	8.202	1.00	17.80	A
35	ATOM C	450	CA	LEU	A	178	188.742	184.695	9.532	1.00	17.25	A
	ATOM C	451	CB	LEU	A	178	189.473	185.495	10.616	1.00	14.48	A
	ATOM C	452	CG	LEU	A	178	188.948	185.297	12.041	1.00	14.78	A
40	ATOM C	453	CD1	LEU	A	178	188.822	183.792	12.391	1.00	13.65	A
	ATOM C	454	CD2	LEU	A	178	189.904	185.964	13.002	1.00	15.52	A
45	ATOM C	455	C	LEU	A	178	187.257	185.050	9.569	1.00	18.82	A
	ATOM O	456	O	LEU	A	178	186.436	184.346	10.148	1.00	18.56	A
	ATOM N	457	N	ARG	A	179	186.929	186.171	8.950	1.00	17.14	A
50	ATOM C	458	CA	ARG	A	179	185.570	186.637	8.893	1.00	20.36	A
	ATOM C	459	CB	ARG	A	179	185.547	188.004	8.238	1.00	24.60	A
55	ATOM C	460	CG	ARG	A	179	184.191	188.581	8.190	1.00	30.51	A
	ATOM C	461	CD	ARG	A	179	184.079	189.355	6.937	1.00	34.92	A
	ATOM N	462	NE	ARG	A	179	183.602	190.700	7.192	1.00	44.42	A
60	ATOM C	463	CZ	ARG	A	179	184.338	191.679	7.721	1.00	50.64	A
	ATOM N	464	NH1	ARG	A	179	185.609	191.475	8.060	1.00	53.62	A

	ATOM N	465	NH2	ARG A	179	183.800	192.881	7.910	1.00	54.27	A
	ATOM C	466	C	ARG A	179	184.677	185.663	8.112	1.00	20.68	A
5	ATOM O	467	O	ARG A	179	183.516	185.428	8.490	1.00	20.49	A
	ATOM N	468	N	ARG A	180	185.211	185.102	7.027	1.00	16.87	A
10	ATOM C	469	CA	ARG A	180	184.457	184.139	6.240	1.00	16.27	A
	ATOM C	470	CB	ARG A	180	185.145	183.851	4.880	1.00	15.64	A
	ATOM C	471	CG	ARG A	180	185.036	184.997	3.869	1.00	19.03	A
15	ATOM C	472	CD	ARG A	180	185.243	184.593	2.394	1.00	19.17	A
	ATOM N	473	NE	ARG A	180	186.536	183.973	2.158	1.00	22.25	A
20	ATOM C	474	CZ	ARG A	180	187.223	184.003	1.011	1.00	22.42	A
	ATOM N	475	NH1	ARG A	180	186.778	184.633	-0.067	1.00	16.67	A
	ATOM N	476	NH2	ARG A	180	188.390	183.384	0.949	1.00	23.03	A
25	ATOM C	477	C	ARG A	180	184.277	182.837	7.037	1.00	16.14	A
	ATOM O	478	O	ARG A	180	183.225	182.207	6.950	1.00	17.78	A
30	ATOM N	479	N	GLU A	181	185.294	182.439	7.812	1.00	15.13	A
	ATOM C	480	CA	GLU A	181	185.211	181.222	8.627	1.00	15.82	A
	ATOM C	481	CB	GLU A	181	186.512	180.969	9.431	1.00	17.60	A
35	ATOM C	482	CG	GLU A	181	186.517	179.610	10.164	1.00	22.11	A
	ATOM C	483	CD	GLU A	181	187.779	179.293	11.023	1.00	29.50	A
40	ATOM O	484	OE1	GLU A	181	188.877	179.898	10.811	1.00	23.91	A
	ATOM O	485	OE2	GLU A	181	187.654	178.393	11.914	1.00	30.52	A
	ATOM C	486	C	GLU A	181	184.059	181.374	9.615	1.00	17.24	A
45	ATOM O	487	O	GLU A	181	183.169	180.514	9.711	1.00	17.81	A
	ATOM N	488	N	VAL A	182	184.075	182.486	10.336	1.00	13.24	A
50	ATOM C	489	CA	VAL A	182	183.056	182.746	11.323	1.00	16.10	A
	ATOM C	490	CB	VAL A	182	183.417	183.989	12.155	1.00	17.20	A
	ATOM C	491	CG1	VAL A	182	182.271	184.362	13.059	1.00	11.33	A
55	ATOM C	492	CG2	VAL A	182	184.675	183.709	12.948	1.00	15.06	A
	ATOM C	493	C	VAL A	182	181.650	182.907	10.756	1.00	16.14	A
60	ATOM O	494	O	VAL A	182	180.718	182.216	11.186	1.00	14.19	A
	ATOM N	495	N	GLU A	183	181.491	183.805	9.788	1.00	16.25	A

	ATOM C	496	CA	GLU A 183	180.162	184.021	9.212	1.00	17.30	A
	ATOM C	497	CB	GLU A 183	180.190	185.187	8.214	1.00	16.51	A
5	ATOM C	498	CG	GLU A 183	180.630	186.499	8.842	1.00	21.63	A
	ATOM C	499	CD	GLU A 183	180.566	187.674	7.874	1.00	24.47	A
10	ATOM O	500	OE1	GLU A 183	180.841	187.477	6.673	1.00	27.21	A
	ATOM O	501	OE2	GLU A 183	180.255	188.801	8.315	1.00	29.43	A
	ATOM C	502	C	GLU A 183	179.581	182.764	8.555	1.00	14.99	A
15	ATOM O	503	O	GLU A 183	178.405	182.460	8.753	1.00	16.33	A
	ATOM N	504	N	ILE A 184	180.396	182.019	7.810	1.00	12.00	A
20	ATOM C	505	CA	ILE A 184	179.908	180.808	7.159	1.00	10.45	A
	ATOM C	506	CB	ILE A 184	180.904	180.302	6.094	1.00	9.02	A
	ATOM C	507	CG2	ILE A 184	180.595	178.854	5.712	1.00	2.93	A
25	ATOM C	508	CG1	ILE A 184	180.862	181.248	4.893	1.00	4.36	A
	ATOM C	509	CD1	ILE A 184	182.025	181.076	3.939	1.00	5.66	A
30	ATOM C	510	C	ILE A 184	179.633	179.675	8.149	1.00	12.74	A
	ATOM O	511	O	ILE A 184	178.552	179.077	8.135	1.00	13.03	A
	ATOM N	512	N	GLN A 185	180.585	179.380	9.026	1.00	14.41	A
35	ATOM C	513	CA	GLN A 185	180.365	178.279	9.960	1.00	15.94	A
	ATOM C	514	CB	GLN A 185	181.663	177.933	10.682	1.00	15.68	A
40	ATOM C	515	CG	GLN A 185	181.684	176.556	11.281	1.00	15.22	A
	ATOM C	516	CD	GLN A 185	182.955	176.333	12.074	1.00	16.62	A
	ATOM O	517	OE1	GLN A 185	183.844	177.184	12.072	1.00	19.84	A
45	ATOM N	518	NE2	GLN A 185	183.048	175.198	12.760	1.00	15.50	A
	ATOM C	519	C	GLN A 185	179.257	178.551	10.977	1.00	14.85	A
50	ATOM O	520	O	GLN A 185	178.507	177.637	11.339	1.00	11.63	A
	ATOM N	521	N	SER A 186	179.134	179.798	11.424	1.00	14.21	A
	ATOM C	522	CA	SER A 186	178.102	180.102	12.421	1.00	15.30	A
55	ATOM C	523	CB	SER A 186	178.265	181.527	13.028	1.00	15.24	A
	ATOM O	524	OG	SER A 186	178.146	182.584	12.086	1.00	16.11	A
60	ATOM C	525	C	SER A 186	176.686	179.916	11.898	1.00	15.48	A
	ATOM O	526	O	SER A 186	175.787	179.612	12.672	1.00	20.12	A

5	10	15	20	25	30	35	40	45	50	55	60
ATOM N	527	N	HIS	A	187	176.483	180.048	10.592	1.00	15.79	A
ATOM C	528	CA	HIS	A	187	175.153	179.908	10.018	1.00	15.76	A
ATOM C	529	CB	HIS	A	187	174.964	180.942	8.914	1.00	14.22	A
ATOM C	530	CG	HIS	A	187	174.857	182.348	9.414	1.00	14.55	A
ATOM C	531	CD2	HIS	A	187	173.787	183.070	9.816	1.00	12.55	A
ATOM N	532	ND1	HIS	A	187	175.944	183.189	9.516	1.00	13.11	A
ATOM C	533	CE1	HIS	A	187	175.548	184.369	9.951	1.00	10.14	A
ATOM N	534	NE2	HIS	A	187	174.243	184.324	10.140	1.00	15.06	A
ATOM C	535	C	HIS	A	187	174.838	178.515	9.469	1.00	17.67	A
ATOM O	536	O	HIS	A	187	173.762	178.272	8.931	1.00	17.40	A
ATOM N	537	N	LEU	A	188	175.777	177.595	9.616	1.00	18.89	A
ATOM C	538	CA	LEU	A	188	175.608	176.243	9.118	1.00	16.21	A
ATOM C	539	CB	LEU	A	188	176.972	175.721	8.652	1.00	15.40	A
ATOM C	540	CG	LEU	A	188	177.339	175.433	7.185	1.00	14.79	A
ATOM C	541	CD1	LEU	A	188	176.514	176.200	6.155	1.00	14.64	A
ATOM C	542	CD2	LEU	A	188	178.805	175.738	7.024	1.00	11.29	A
ATOM C	543	C	LEU	A	188	175.047	175.408	10.266	1.00	17.59	A
ATOM O	544	O	LEU	A	188	175.382	175.630	11.423	1.00	19.21	A
ATOM N	545	N	ARG	A	189	174.174	174.458	9.955	1.00	19.36	A
ATOM C	546	CA	ARG	A	189	173.579	173.603	10.988	1.00	21.36	A
ATOM C	547	CB	ARG	A	189	172.190	174.086	11.398	1.00	22.58	A
ATOM C	548	CG	ARG	A	189	172.131	175.420	12.110	1.00	32.57	A
ATOM C	549	CD	ARG	A	189	172.277	175.274	13.621	1.00	34.83	A
ATOM N	550	NE	ARG	A	189	172.168	176.568	14.298	1.00	40.56	A
ATOM C	551	CZ	ARG	A	189	172.993	177.598	14.091	1.00	43.35	A
ATOM N	552	NH1	ARG	A	189	173.993	177.481	13.215	1.00	42.31	A
ATOM N	553	NH2	ARG	A	189	172.827	178.740	14.770	1.00	42.32	A
ATOM C	554	C	ARG	A	189	173.423	172.219	10.415	1.00	19.45	A
ATOM O	555	O	ARG	A	189	172.582	171.996	9.558	1.00	19.37	A
ATOM N	556	N	HIS	A	190	174.218	171.283	10.900	1.00	16.48	A
ATOM C	557	CA	HIS	A	190	174.148	169.936	10.388	1.00	16.32	A

5	ATOM C	558	CB	HIS	A	190	174.865	169.868	9.042	1.00	13.06	A
	ATOM C	559	CG	HIS	A	190	174.848	168.517	8.403	1.00	8.96	A
	ATOM C	560	CD2	HIS	A	190	175.640	167.430	8.584	1.00	9.19	A
	ATOM N	561	ND1	HIS	A	190	173.942	168.169	7.422	1.00	9.60	A
10	ATOM C	562	CE1	HIS	A	190	174.177	166.929	7.026	1.00	8.25	A
	ATOM N	563	NE2	HIS	A	190	175.202	166.456	7.717	1.00	10.48	A
15	ATOM C	564	C	HIS	A	190	174.857	169.069	11.409	1.00	18.77	A
	ATOM O	565	O	HIS	A	190	175.747	169.538	12.110	1.00	19.58	A
20	ATOM N	566	N	PRO	A	191	174.437	167.797	11.526	1.00	19.81	A
	ATOM C	567	CD	PRO	A	191	173.236	167.329	10.808	1.00	18.67	A
	ATOM C	568	CA	PRO	A	191	174.946	166.749	12.430	1.00	18.82	A
25	ATOM C	569	CB	PRO	A	191	174.058	165.545	12.108	1.00	15.98	A
	ATOM C	570	CG	PRO	A	191	172.813	166.147	11.615	1.00	19.49	A
30	ATOM C	571	C	PRO	A	191	176.422	166.383	12.239	1.00	15.63	A
	ATOM O	572	O	PRO	A	191	177.074	165.908	13.167	1.00	16.18	A
	ATOM N	573	N	ASN	A	192	176.930	166.564	11.029	1.00	13.38	A
35	ATOM C	574	CA	ASN	A	192	178.306	166.216	10.740	1.00	13.06	A
	ATOM C	575	CB	ASN	A	192	178.367	165.242	9.568	1.00	16.94	A
40	ATOM C	576	CG	ASN	A	192	177.621	163.963	9.853	1.00	21.40	A
	ATOM O	577	OD1	ASN	A	192	176.478	163.790	9.431	1.00	24.81	A
	ATOM N	578	ND2	ASN	A	192	178.255	163.062	10.596	1.00	19.25	A
45	ATOM C	579	C	ASN	A	192	179.189	167.407	10.467	1.00	13.65	A
	ATOM O	580	O	ASN	A	192	180.258	167.276	9.869	1.00	15.58	A
50	ATOM N	581	N	ILE	A	193	178.725	168.584	10.865	1.00	13.34	A
	ATOM C	582	CA	ILE	A	193	179.529	169.789	10.734	1.00	12.06	A
	ATOM C	583	CB	ILE	A	193	178.886	170.843	9.814	1.00	11.35	A
55	ATOM C	584	CG2	ILE	A	193	179.688	172.131	9.882	1.00	5.81	A
	ATOM C	585	CG1	ILE	A	193	178.807	170.317	8.381	1.00	6.17	A
60	ATOM C	586	CD1	ILE	A	193	178.045	171.205	7.453	1.00	8.69	A
	ATOM C	587	C	ILE	A	193	179.651	170.377	12.134	1.00	12.85	A
	ATOM O	588	O	ILE	A	193	178.663	170.540	12.840	1.00	14.90	A

5	ATOM N	589	N	LEU A 194	180.874	170.678	12.530	1.00	13.66	A
	ATOM C	590	CA	LEU A 194	181.123	171.253	13.839	1.00	14.76	A
	ATOM C	591	CB	LEU A 194	182.623	171.519	14.036	1.00	16.68	A
	ATOM C	592	CG	LEU A 194	183.117	171.537	15.486	1.00	15.84	A
10	ATOM C	593	CD1	LEU A 194	183.039	170.099	16.000	1.00	14.02	A
	ATOM C	594	CD2	LEU A 194	184.545	172.073	15.588	1.00	14.49	A
15	ATOM C	595	C	LEU A 194	180.381	172.578	13.964	1.00	16.81	A
	ATOM O	596	O	LEU A 194	180.450	173.433	13.070	1.00	18.34	A
20	ATOM N	597	N	ARG A 195	179.683	172.727	15.085	1.00	15.08	A
	ATOM C	598	CA	ARG A 195	178.924	173.924	15.390	1.00	16.45	A
	ATOM C	599	CB	ARG A 195	177.878	173.634	16.474	1.00	19.44	A
25	ATOM C	600	CG	ARG A 195	176.596	172.975	15.987	1.00	25.93	A
	ATOM C	601	CD	ARG A 195	175.746	173.967	15.232	1.00	29.82	A
30	ATOM N	602	NE	ARG A 195	174.811	174.694	16.091	1.00	36.41	A
	ATOM C	603	CZ	ARG A 195	174.859	176.008	16.302	1.00	39.91	A
	ATOM N	604	NH1	ARG A 195	175.804	176.729	15.718	1.00	44.61	A
	ATOM N	605	NH2	ARG A 195	173.958	176.608	17.075	1.00	40.14	A
35	ATOM C	606	C	ARG A 195	179.787	175.113	15.870	1.00	16.17	A
	ATOM O	607	O	ARG A 195	180.714	174.950	16.656	1.00	13.03	A
40	ATOM N	608	N	LEU A 196	179.471	176.293	15.341	1.00	17.85	A
	ATOM C	609	CA	LEU A 196	180.114	177.536	15.749	1.00	16.50	A
45	ATOM C	610	CB	LEU A 196	180.623	178.380	14.572	1.00	13.17	A
	ATOM C	611	CG	LEU A 196	181.348	179.669	14.959	1.00	15.31	A
	ATOM C	612	CD1	LEU A 196	182.467	179.277	15.910	1.00	13.98	A
50	ATOM C	613	CD2	LEU A 196	181.922	180.404	13.749	1.00	12.29	A
	ATOM C	614	C	LEU A 196	178.975	178.281	16.466	1.00	15.90	A
55	ATOM O	615	O	LEU A 196	178.037	178.767	15.839	1.00	15.06	A
	ATOM N	616	N	TYR A 197	179.062	178.337	17.791	1.00	18.19	A
60	ATOM C	617	CA	TYR A 197	178.049	178.974	18.610	1.00	18.38	A
	ATOM C	618	CB	TYR A 197	178.154	178.464	20.033	1.00	15.79	A
	ATOM C	619	CG	TYR A 197	177.908	176.980	20.126	1.00	17.64	A

5	ATOM C	620	CD1	TYR	A	197	178.955	176.080	20.280	1.00	15.26	A
	ATOM C	621	CE1	TYR	A	197	178.712	174.718	20.364	1.00	20.64	A
	ATOM C	622	CD2	TYR	A	197	176.607	176.469	20.054	1.00	21.32	A
	ATOM C	623	CE2	TYR	A	197	176.360	175.104	20.138	1.00	20.23	A
10	ATOM C	624	CZ	TYR	A	197	177.418	174.242	20.293	1.00	20.94	A
	ATOM O	625	OH	TYR	A	197	177.185	172.900	20.387	1.00	26.42	A
15	ATOM C	626	C	TYR	A	197	178.174	180.481	18.561	1.00	19.88	A
	ATOM O	627	O	TYR	A	197	177.180	181.193	18.454	1.00	19.95	A
	ATOM N	628	N	GLY	A	198	179.394	180.985	18.611	1.00	20.35	A
20	ATOM C	629	CA	GLY	A	198	179.542	182.425	18.562	1.00	20.00	A
	ATOM C	630	C	GLY	A	198	180.984	182.838	18.642	1.00	17.90	A
25	ATOM O	631	O	GLY	A	198	181.874	182.005	18.677	1.00	19.17	A
	ATOM N	632	N	TYR	A	199	181.222	184.134	18.686	1.00	17.72	A
	ATOM C	633	CA	TYR	A	199	182.589	184.593	18.748	1.00	19.93	A
30	ATOM C	634	CB	TYR	A	199	183.128	184.776	17.325	1.00	19.83	A
	ATOM C	635	CG	TYR	A	199	182.894	186.166	16.788	1.00	21.41	A
35	ATOM C	636	CD1	TYR	A	199	183.892	187.135	16.885	1.00	21.65	A
	ATOM C	637	CE1	TYR	A	199	183.677	188.430	16.486	1.00	22.65	A
	ATOM C	638	CD2	TYR	A	199	181.660	186.538	16.266	1.00	18.59	A
40	ATOM C	639	CE2	TYR	A	199	181.426	187.841	15.862	1.00	22.04	A
	ATOM C	640	CZ	TYR	A	199	182.439	188.787	15.972	1.00	23.54	A
45	ATOM O	641	OH	TYR	A	199	182.223	190.089	15.557	1.00	24.04	A
	ATOM C	642	C	TYR	A	199	182.693	185.910	19.508	1.00	19.03	A
	ATOM O	643	O	TYR	A	199	181.703	186.618	19.699	1.00	19.48	A
50	ATOM N	644	N	PHE	A	200	183.910	186.238	19.920	1.00	18.13	A
	ATOM C	645	CA	PHE	A	200	184.177	187.478	20.627	1.00	17.58	A
55	ATOM C	646	CB	PHE	A	200	183.677	187.397	22.091	1.00	12.35	A
	ATOM C	647	CG	PHE	A	200	184.369	186.344	22.955	1.00	13.81	A
	ATOM C	648	CD1	PHE	A	200	185.449	186.685	23.779	1.00	14.44	A
60	ATOM C	649	CD2	PHE	A	200	183.898	185.033	22.998	1.00	12.16	A
	ATOM C	650	CE1	PHE	A	200	186.043	185.731	24.636	1.00	13.44	A

5	ATOM C	651	CE2	PHE	A	200	184.474	184.075	23.845	1.00	13.42	A
	ATOM C	652	CZ	PHE	A	200	185.552	184.426	24.669	1.00	13.28	A
	ATOM C	653	C	PHE	A	200	185.675	187.756	20.549	1.00	18.86	A
	ATOM O	654	O	PHE	A	200	186.482	186.840	20.451	1.00	24.13	A
10	ATOM N	655	N	HIS	A	201	186.056	189.019	20.573	1.00	19.06	A
	ATOM C	656	CA	HIS	A	201	187.467	189.335	20.512	1.00	22.05	A
15	ATOM C	657	CB	HIS	A	201	187.820	189.966	19.159	1.00	20.51	A
	ATOM C	658	CG	HIS	A	201	187.161	191.286	18.903	1.00	18.99	A
20	ATOM C	659	CD2	HIS	A	201	185.922	191.593	18.450	1.00	19.83	A
	ATOM N	660	ND1	HIS	A	201	187.848	192.478	18.965	1.00	21.28	A
	ATOM C	661	CE1	HIS	A	201	187.071	193.459	18.544	1.00	19.32	A
25	ATOM N	662	NE2	HIS	A	201	185.896	192.948	18.223	1.00	20.12	A
	ATOM C	663	C	HIS	A	201	187.840	190.279	21.629	1.00	22.96	A
30	ATOM O	664	O	HIS	A	201	186.977	190.871	22.253	1.00	23.67	A
	ATOM N	665	N	ASP	A	202	189.126	190.395	21.913	1.00	23.03	A
	ATOM C	666	CA	ASP	A	202	189.535	191.331	22.936	1.00	24.25	A
35	ATOM C	667	CB	ASP	A	202	189.928	190.621	24.235	1.00	25.39	A
	ATOM C	668	CG	ASP	A	202	191.175	189.780	24.097	1.00	28.38	A
40	ATOM O	669	OD1	ASP	A	202	191.836	189.826	23.031	1.00	34.60	A
	ATOM O	670	OD2	ASP	A	202	191.495	189.066	25.067	1.00	24.71	A
	ATOM C	671	C	ASP	A	202	190.696	192.148	22.398	1.00	25.07	A
45	ATOM O	672	O	ASP	A	202	190.896	192.235	21.193	1.00	24.05	A
	ATOM N	673	N	ALA	A	203	191.480	192.733	23.287	1.00	26.38	A
50	ATOM C	674	CA	ALA	A	203	192.595	193.564	22.856	1.00	25.39	A
	ATOM C	675	CB	ALA	A	203	193.217	194.257	24.082	1.00	23.30	A
	ATOM C	676	C	ALA	A	203	193.678	192.847	22.039	1.00	25.31	A
55	ATOM O	677	O	ALA	A	203	194.184	193.405	21.070	1.00	24.76	A
	ATOM N	678	N	THR	A	204	194.038	191.623	22.409	1.00	24.17	A
60	ATOM C	679	CA	THR	A	204	195.084	190.922	21.682	1.00	24.93	A
	ATOM C	680	CB	THR	A	204	196.202	190.467	22.631	1.00	28.17	A
	ATOM O	681	OG1	THR	A	204	195.667	189.534	23.582	1.00	29.58	A

5	ATOM C	682	CG2	THR	A	204	196.805	191.672	23.364	1.00	26.38	A
	ATOM C	683	C	THR	A	204	194.638	189.711	20.869	1.00	26.55	A
10	ATOM O	684	O	THR	A	204	195.360	189.270	19.968	1.00	25.70	A
	ATOM N	685	N	ARG	A	205	193.469	189.149	21.166	1.00	26.89	A
15	ATOM C	686	CA	ARG	A	205	193.039	188.002	20.382	1.00	26.09	A
	ATOM C	687	CB	ARG	A	205	193.558	186.710	21.026	1.00	29.89	A
20	ATOM C	688	CG	ARG	A	205	193.403	186.595	22.508	1.00	35.65	A
	ATOM C	689	CD	ARG	A	205	194.768	186.465	23.174	1.00	41.67	A
25	ATOM N	690	NE	ARG	A	205	194.650	186.517	24.630	1.00	50.08	A
	ATOM C	691	CZ	ARG	A	205	195.657	186.756	25.467	1.00	53.61	A
30	ATOM N	692	NH1	ARG	A	205	196.884	186.972	24.997	1.00	54.63	A
	ATOM N	693	NH2	ARG	A	205	195.429	186.782	26.781	1.00	57.41	A
35	ATOM C	694	C	ARG	A	205	191.561	187.869	20.036	1.00	23.76	A
	ATOM O	695	O	ARG	A	205	190.728	188.654	20.478	1.00	26.35	A
40	ATOM N	696	N	VAL	A	206	191.253	186.892	19.187	1.00	21.67	A
	ATOM C	697	CA	VAL	A	206	189.883	186.606	18.776	1.00	17.07	A
45	ATOM C	698	CB	VAL	A	206	189.704	186.683	17.247	1.00	16.64	A
	ATOM C	699	CG1	VAL	A	206	188.235	186.422	16.888	1.00	11.75	A
50	ATOM C	700	CG2	VAL	A	206	190.136	188.055	16.741	1.00	15.29	A
	ATOM C	701	C	VAL	A	206	189.541	185.179	19.225	1.00	16.35	A
55	ATOM O	702	O	VAL	A	206	190.380	184.277	19.146	1.00	15.34	A
	ATOM N	703	N	TYR	A	207	188.308	184.987	19.688	1.00	15.70	A
60	ATOM C	704	CA	TYR	A	207	187.866	183.692	20.185	1.00	14.78	A
	ATOM C	705	CB	TYR	A	207	187.555	183.754	21.686	1.00	14.30	A
65	ATOM C	706	CG	TYR	A	207	188.599	184.415	22.538	1.00	15.34	A
	ATOM C	707	CD1	TYR	A	207	188.725	185.809	22.565	1.00	15.56	A
70	ATOM C	708	CE1	TYR	A	207	189.669	186.433	23.389	1.00	14.72	A
	ATOM C	709	CD2	TYR	A	207	189.445	183.655	23.347	1.00	13.39	A
75	ATOM C	710	CE2	TYR	A	207	190.393	184.263	24.174	1.00	15.70	A
	ATOM C	711	CZ	TYR	A	207	190.497	185.652	24.192	1.00	16.96	A
80	ATOM O	712	OH	TYR	A	207	191.413	186.252	25.028	1.00	17.44	A

5	ATOM C	713	C	TYR A 207	186.624	183.132	19.506	1.00	14.64	A
	ATOM O	714	O	TYR A 207	185.604	183.807	19.390	1.00	14.86	A
	ATOM N	715	N	LEU A 208	186.716	181.882	19.082	1.00	12.98	A
	ATOM C	716	CA	LEU A 208	185.597	181.206	18.475	1.00	11.35	A
10	ATOM C	717	CB	LEU A 208	186.025	180.515	17.181	1.00	12.38	A
	ATOM C	718	CG	LEU A 208	186.790	181.296	16.101	1.00	18.53	A
15	ATOM C	719	CD1	LEU A 208	186.415	180.695	14.759	1.00	13.01	A
	ATOM C	720	CD2	LEU A 208	186.466	182.794	16.118	1.00	17.18	A
20	ATOM C	721	C	LEU A 208	185.092	180.162	19.473	1.00	11.42	A
	ATOM O	722	O	LEU A 208	185.875	179.354	19.978	1.00	9.69	A
	ATOM N	723	N	ILE A 209	183.789	180.194	19.753	1.00	11.10	A
	ATOM C	724	CA	ILE A 209	183.146	179.268	20.670	1.00	10.69	A
25	ATOM C	725	CB	ILE A 209	181.968	179.962	21.389	1.00	13.97	A
	ATOM C	726	CG2	ILE A 209	181.316	178.980	22.422	1.00	10.28	A
30	ATOM C	727	CG1	ILE A 209	182.489	181.303	21.979	1.00	14.77	A
	ATOM C	728	CD1	ILE A 209	181.466	182.209	22.621	1.00	10.27	A
35	ATOM C	729	C	ILE A 209	182.659	178.124	19.785	1.00	13.02	A
	ATOM O	730	O	ILE A 209	181.689	178.238	19.040	1.00	13.94	A
	ATOM N	731	N	LEU A 210	183.373	177.019	19.856	1.00	12.66	A
	ATOM C	732	CA	LEU A 210	183.065	175.867	19.044	1.00	13.21	A
40	ATOM C	733	CB	LEU A 210	184.348	175.383	18.375	1.00	13.93	A
	ATOM C	734	CG	LEU A 210	185.046	176.317	17.381	1.00	16.57	A
45	ATOM C	735	CD1	LEU A 210	186.507	175.915	17.264	1.00	14.44	A
	ATOM C	736	CD2	LEU A 210	184.351	176.245	16.022	1.00	12.75	A
50	ATOM C	737	C	LEU A 210	182.464	174.731	19.841	1.00	10.33	A
	ATOM O	738	O	LEU A 210	182.591	174.664	21.053	1.00	14.25	A
55	ATOM N	739	N	GLU A 211	181.784	173.843	19.139	1.00	11.52	A
	ATOM C	740	CA	GLU A 211	181.218	172.646	19.739	1.00	12.06	A
60	ATOM C	741	CB	GLU A 211	180.272	171.970	18.751	1.00	15.25	A
	ATOM C	742	CG	GLU A 211	180.147	170.462	18.927	1.00	16.63	A
	ATOM C	743	CD	GLU A 211	179.379	169.783	17.784	1.00	23.31	A

5	ATOM O	744	OE1	GLU	A	211	179.201	168.531	17.837	1.00	22.59	A
	ATOM O	745	OE2	GLU	A	211	178.954	170.500	16.829	1.00	22.15	A
	ATOM C	746	C	GLU	A	211	182.424	171.723	20.009	1.00	14.58	A
	ATOM O	747	O	GLU	A	211	183.296	171.561	19.156	1.00	11.41	A
10	ATOM N	748	N	TYR	A	212	182.466	171.133	21.196	1.00	13.40	A
	ATOM C	749	CA	TYR	A	212	183.555	170.247	21.589	1.00	15.01	A
15	ATOM C	750	CB	TYR	A	212	183.541	170.072	23.108	1.00	16.32	A
	ATOM C	751	CG	TYR	A	212	184.387	168.938	23.679	1.00	18.16	A
	ATOM C	752	CD1	TYR	A	212	185.744	168.820	23.391	1.00	15.83	A
20	ATOM C	753	CE1	TYR	A	212	186.528	167.845	24.013	1.00	16.35	A
	ATOM C	754	CD2	TYR	A	212	183.829	168.042	24.601	1.00	18.49	A
25	ATOM C	755	CE2	TYR	A	212	184.590	167.074	25.223	1.00	16.40	A
	ATOM C	756	CZ	TYR	A	212	185.934	166.973	24.934	1.00	19.22	A
	ATOM O	757	OH	TYR	A	212	186.655	165.995	25.594	1.00	15.81	A
30	ATOM C	758	C	TYR	A	212	183.463	168.889	20.909	1.00	15.14	A
	ATOM O	759	O	TYR	A	212	182.414	168.259	20.920	1.00	14.66	A
35	ATOM N	760	N	ALA	A	213	184.561	168.451	20.297	1.00	15.74	A
	ATOM C	761	CA	ALA	A	213	184.623	167.142	19.636	1.00	14.66	A
	ATOM C	762	CB	ALA	A	213	185.341	167.270	18.302	1.00	16.59	A
40	ATOM C	763	C	ALA	A	213	185.417	166.270	20.615	1.00	16.61	A
	ATOM O	764	O	ALA	A	213	186.638	166.352	20.682	1.00	16.21	A
45	ATOM N	765	N	PRO	A	214	184.724	165.418	21.380	1.00	15.97	A
	ATOM C	766	CD	PRO	A	214	183.323	165.077	21.082	1.00	15.58	A
	ATOM C	767	CA	PRO	A	214	185.258	164.515	22.398	1.00	15.31	A
50	ATOM C	768	CB	PRO	A	214	184.000	163.837	22.963	1.00	14.60	A
	ATOM C	769	CG	PRO	A	214	182.844	164.624	22.417	1.00	17.26	A
55	ATOM C	770	C	PRO	A	214	186.319	163.472	22.000	1.00	17.90	A
	ATOM O	771	O	PRO	A	214	187.172	163.152	22.829	1.00	18.00	A
	ATOM N	772	N	LEU	A	215	186.274	162.922	20.777	1.00	14.95	A
60	ATOM C	773	CA	LEU	A	215	187.214	161.880	20.362	1.00	14.66	A
	ATOM C	774	CB	LEU	A	215	186.453	160.710	19.692	1.00	16.00	A

5	ATOM C	775	CG	LEU	A	215	185.316	160.072	20.536	1.00	22.00	A
	ATOM C	776	CD1	LEU	A	215	184.664	158.818	19.898	1.00	17.85	A
	ATOM C	777	CD2	LEU	A	215	185.906	159.717	21.877	1.00	20.55	A
	ATOM C	778	C	LEU	A	215	188.415	162.306	19.505	1.00	14.59	A
	ATOM O	779	O	LEU	A	215	189.093	161.477	18.905	1.00	14.29	A
10	ATOM N	780	N	GLY	A	216	188.691	163.603	19.455	1.00	16.74	A
	ATOM C	781	CA	GLY	A	216	189.836	164.070	18.694	1.00	14.83	A
15	ATOM C	782	C	GLY	A	216	189.701	164.060	17.184	1.00	13.54	A
	ATOM O	783	O	GLY	A	216	188.597	164.008	16.656	1.00	12.48	A
20	ATOM N	784	N	THR	A	217	190.843	164.091	16.497	1.00	12.97	A
	ATOM C	785	CA	THR	A	217	190.867	164.136	15.044	1.00	14.08	A
25	ATOM C	786	CB	THR	A	217	192.005	164.998	14.503	1.00	14.49	A
	ATOM O	787	OG1	THR	A	217	193.242	164.310	14.733	1.00	16.68	A
30	ATOM C	788	CG2	THR	A	217	192.043	166.347	15.167	1.00	10.84	A
	ATOM C	789	C	THR	A	217	191.060	162.811	14.347	1.00	16.46	A
35	ATOM O	790	O	THR	A	217	191.741	161.910	14.849	1.00	15.02	A
	ATOM N	791	N	VAL	A	218	190.481	162.721	13.153	1.00	16.27	A
40	ATOM C	792	CA	VAL	A	218	190.616	161.533	12.340	1.00	15.99	A
	ATOM C	793	CB	VAL	A	218	189.802	161.683	11.038	1.00	16.57	A
45	ATOM C	794	CG1	VAL	A	218	190.263	160.649	9.999	1.00	18.56	A
	ATOM C	795	CG2	VAL	A	218	188.339	161.504	11.349	1.00	11.27	A
50	ATOM C	796	C	VAL	A	218	192.117	161.366	12.051	1.00	16.41	A
	ATOM O	797	O	VAL	A	218	192.611	160.255	11.896	1.00	15.84	A
55	ATOM N	798	N	TYR	A	219	192.826	162.487	12.008	1.00	15.85	A
	ATOM C	799	CA	TYR	A	219	194.261	162.509	11.789	1.00	16.76	A
60	ATOM C	800	CB	TYR	A	219	194.771	163.937	11.908	1.00	18.52	A
	ATOM C	801	CG	TYR	A	219	196.259	164.024	11.800	1.00	19.33	A
65	ATOM C	802	CD1	TYR	A	219	196.870	163.870	10.570	1.00	17.55	A
	ATOM C	803	CE1	TYR	A	219	198.249	163.929	10.450	1.00	23.59	A
70	ATOM C	804	CD2	TYR	A	219	197.065	164.236	12.936	1.00	21.27	A
	ATOM C	805	CE2	TYR	A	219	198.454	164.289	12.834	1.00	20.92	A

	ATOM	806	CZ	TYR A 219	199.032	164.136	11.584	1.00	24.53	A
	ATOM C	807	OH	TYR A 219	200.392	164.188	11.448	1.00	28.22	A
5	O ATOM	808	C	TYR A 219	194.999	161.661	12.826	1.00	18.49	A
	ATOM O	809	O	TYR A 219	195.910	160.888	12.494	1.00	18.32	A
10	ATOM N	810	N	ARG A 220	194.617	161.836	14.086	1.00	16.66	A
	ATOM C	811	CA	ARG A 220	195.247	161.100	15.154	1.00	19.76	A
	ATOM C	812	CB	ARG A 220	194.848	161.674	16.514	1.00	22.26	A
15	ATOM C	813	CG	ARG A 220	195.514	160.949	17.669	1.00	27.26	A
	ATOM C	814	CD	ARG A 220	197.039	161.124	17.660	1.00	29.11	A
20	ATOM N	815	NE	ARG A 220	197.689	160.200	18.595	1.00	32.84	A
	ATOM C	816	CZ	ARG A 220	199.003	160.005	18.702	1.00	35.53	A
	ATOM N	817	NH1	ARG A 220	199.867	160.669	17.931	1.00	39.53	A
25	ATOM N	818	NH2	ARG A 220	199.449	159.129	19.594	1.00	36.11	A
	ATOM C	819	C	ARG A 220	194.908	159.608	15.088	1.00	19.85	A
30	ATOM O	820	O	ARG A 220	195.768	158.748	15.322	1.00	19.84	A
	ATOM N	821	N	GLU A 221	193.661	159.309	14.746	1.00	19.44	A
	ATOM C	822	CA	GLU A 221	193.192	157.935	14.628	1.00	21.14	A
35	ATOM C	823	CB	GLU A 221	191.670	157.930	14.386	1.00	22.94	A
	ATOM C	824	CG	GLU A 221	190.968	156.594	14.519	1.00	27.24	A
40	ATOM C	825	CD	GLU A 221	191.078	155.998	15.918	1.00	30.92	A
	ATOM O	826	OE1	GLU A 221	190.736	154.798	16.073	1.00	35.57	A
	ATOM O	827	OE2	GLU A 221	191.502	156.716	16.857	1.00	31.40	A
45	ATOM C	828	C	GLU A 221	193.930	157.268	13.465	1.00	22.03	A
	ATOM O	829	O	GLU A 221	194.201	156.061	13.493	1.00	21.79	A
50	ATOM N	830	N	LEU A 222	194.257	158.060	12.442	1.00	20.91	A
	ATOM C	831	CA	LEU A 222	194.969	157.533	11.287	1.00	18.01	A
	ATOM C	832	CB	LEU A 222	194.838	158.485	10.079	1.00	17.83	A
55	ATOM C	833	CG	LEU A 222	195.181	157.923	8.676	1.00	21.87	A
	ATOM C	834	CD1	LEU A 222	194.366	156.652	8.358	1.00	17.44	A
60	ATOM C	835	CD2	LEU A 222	194.892	159.007	7.634	1.00	19.79	A
	ATOM C	836	C	LEU A 222	196.439	157.261	11.639	1.00	16.91	A

5	ATOM O	837	O	LEU	A	222	197.012	156.317	11.119	1.00	16.89	A
	ATOM N	838	N	GLN	A	223	197.062	158.066	12.503	1.00	16.66	A
	ATOM C	839	CA	GLN	A	223	198.446	157.769	12.900	1.00	17.24	A
	ATOM C	840	CB	GLN	A	223	199.022	158.808	13.850	1.00	19.18	A
10	ATOM C	841	CG	GLN	A	223	199.250	160.205	13.317	1.00	28.34	A
	ATOM C	842	CD	GLN	A	223	199.954	161.058	14.355	1.00	31.88	A
15	ATOM O	843	OE1	GLN	A	223	199.437	161.241	15.474	1.00	31.86	A
	ATOM N	844	NE2	GLN	A	223	201.149	161.584	14.005	1.00	34.43	A
	ATOM C	845	C	GLN	A	223	198.456	156.448	13.688	1.00	21.01	A
20	ATOM O	846	O	GLN	A	223	199.360	155.630	13.523	1.00	18.77	A
	ATOM N	847	N	LYS	A	224	197.464	156.277	14.570	1.00	21.30	A
25	ATOM C	848	CA	LYS	A	224	197.357	155.099	15.419	1.00	21.07	A
	ATOM C	849	CB	LYS	A	224	196.258	155.300	16.492	1.00	24.80	A
	ATOM C	850	CG	LYS	A	224	196.479	156.522	17.399	1.00	26.43	A
30	ATOM C	851	CD	LYS	A	224	195.427	156.642	18.505	1.00	30.49	A
	ATOM C	852	CE	LYS	A	224	195.834	157.727	19.507	1.00	31.44	A
35	ATOM N	853	NZ	LYS	A	224	194.917	157.868	20.668	1.00	33.32	A
	ATOM C	854	C	LYS	A	224	197.088	153.812	14.647	1.00	20.29	A
	ATOM O	855	O	LYS	A	224	197.799	152.829	14.821	1.00	19.90	A
40	ATOM N	856	N	LEU	A	225	196.059	153.800	13.806	1.00	20.45	A
	ATOM C	857	CA	LEU	A	225	195.753	152.603	13.039	1.00	18.46	A
45	ATOM C	858	CB	LEU	A	225	194.272	152.588	12.615	1.00	20.03	A
	ATOM C	859	CG	LEU	A	225	193.224	152.691	13.740	1.00	24.89	A
50	ATOM C	860	CD1	LEU	A	225	191.784	152.656	13.213	1.00	20.57	A
	ATOM C	861	CD2	LEU	A	225	193.462	151.543	14.674	1.00	26.58	A
	ATOM C	862	C	LEU	A	225	196.631	152.464	11.780	1.00	19.83	A
	ATOM O	863	O	LEU	A	225	196.694	151.381	11.186	1.00	20.09	A
55	ATOM N	864	N	SER	A	226	197.296	153.545	11.375	1.00	18.33	A
	ATOM C	865	CA	SER	A	226	198.137	153.578	10.158	1.00	21.51	A
60	ATOM C	866	CB	SER	A	226	199.160	152.426	10.124	1.00	21.48	A
	ATOM O	867	OG	SER	A	226	200.116	152.533	11.177	1.00	27.63	A

5	ATOM C	868	C	SER A 226	197.295	153.542	8.871	1.00	20.48	A
	ATOM O	869	O	SER A 226	197.566	154.284	7.927	1.00	19.41	A
	ATOM N	870	N	LYS A 227	196.290	152.664	8.838	1.00	20.02	A
	ATOM C	871	CA	LYS A 227	195.358	152.524	7.697	1.00	19.86	A
10	ATOM C	872	CB	LYS A 227	195.668	151.280	6.876	1.00	24.72	A
	ATOM C	873	CG	LYS A 227	196.854	151.364	5.990	1.00	29.64	A
	ATOM C	874	CD	LYS A 227	197.148	149.990	5.419	1.00	35.21	A
15	ATOM C	875	CE	LYS A 227	198.330	150.088	4.465	1.00	41.32	A
	ATOM N	876	NZ	LYS A 227	198.843	148.758	4.016	1.00	43.82	A
20	ATOM C	877	C	LYS A 227	193.970	152.303	8.274	1.00	16.62	A
	ATOM O	878	O	LYS A 227	193.852	151.881	9.411	1.00	18.80	A
25	ATOM N	879	N	PHE A 228	192.930	152.584	7.499	1.00	14.54	A
	ATOM C	880	CA	PHE A 228	191.548	152.342	7.932	1.00	15.70	A
	ATOM C	881	CB	PHE A 228	190.665	153.590	7.729	1.00	12.09	A
30	ATOM C	882	CG	PHE A 228	190.958	154.697	8.679	1.00	13.97	A
	ATOM C	883	CD1	PHE A 228	190.564	156.005	8.400	1.00	14.03	A
35	ATOM C	884	CD2	PHE A 228	191.629	154.439	9.860	1.00	13.49	A
	ATOM C	885	CE1	PHE A 228	190.844	157.046	9.299	1.00	12.37	A
	ATOM C	886	CE2	PHE A 228	191.912	155.466	10.767	1.00	14.79	A
40	ATOM C	887	CZ	PHE A 228	191.520	156.772	10.487	1.00	11.50	A
	ATOM C	888	C	PHE A 228	191.051	151.227	7.016	1.00	15.70	A
45	ATOM O	889	O	PHE A 228	191.399	151.212	5.833	1.00	16.89	A
	ATOM N	890	N	ASP A 229	190.261	150.290	7.536	1.00	16.61	A
	ATOM C	891	CA	ASP A 229	189.753	149.221	6.666	1.00	18.23	A
50	ATOM C	892	CB	ASP A 229	189.261	148.005	7.478	1.00	17.42	A
	ATOM C	893	CG	ASP A 229	188.092	148.325	8.369	1.00	20.41	A
55	ATOM O	894	OD1	ASP A 229	187.161	149.024	7.930	1.00	28.20	A
	ATOM O	895	OD2	ASP A 229	188.072	147.859	9.511	1.00	26.24	A
	ATOM C	896	C	ASP A 229	188.624	149.817	5.810	1.00	16.57	A
60	ATOM O	897	O	ASP A 229	188.322	151.006	5.939	1.00	17.37	A
	ATOM N	898	N	GLU A 230	187.998	149.020	4.952	1.00	15.33	A

5	ATOM C	899	CA	GLU	A	230	186.947	149.560	4.084	1.00	17.43	A
	ATOM C	900	CB	GLU	A	230	186.571	148.541	3.002	1.00	16.24	A
	ATOM C	901	CG	GLU	A	230	187.743	148.066	2.153	1.00	23.01	A
	ATOM C	902	CD	GLU	A	230	187.313	147.497	0.794	1.00	27.22	A
10	ATOM O	903	OE1	GLU	A	230	186.584	146.478	0.753	1.00	28.49	A
	ATOM O	904	OE2	GLU	A	230	187.711	148.085	-0.244	1.00	29.45	A
15	ATOM C	905	C	GLU	A	230	185.680	150.062	4.783	1.00	16.70	A
	ATOM O	906	O	GLU	A	230	185.141	151.099	4.419	1.00	13.33	A
20	ATOM N	907	N	GLN	A	231	185.209	149.326	5.782	1.00	16.53	A
	ATOM C	908	CA	GLN	A	231	184.003	149.711	6.512	1.00	17.02	A
	ATOM C	909	CB	GLN	A	231	183.728	148.656	7.596	1.00	15.32	A
	ATOM C	910	CG	GLN	A	231	182.370	148.737	8.289	1.00	17.56	A
25	ATOM C	911	CD	GLN	A	231	182.297	149.841	9.359	1.00	22.59	A
	ATOM O	912	OE1	GLN	A	231	183.298	150.112	10.075	1.00	21.11	A
30	ATOM N	913	NE2	GLN	A	231	181.106	150.478	9.494	1.00	19.70	A
	ATOM C	914	C	GLN	A	231	184.195	151.124	7.120	1.00	17.00	A
35	ATOM O	915	O	GLN	A	231	183.381	152.024	6.890	1.00	18.40	A
	ATOM N	916	N	ARG	A	232	185.281	151.308	7.873	1.00	17.36	A
	ATOM C	917	CA	ARG	A	232	185.607	152.593	8.509	1.00	17.63	A
40	ATOM C	918	CB	ARG	A	232	186.905	152.465	9.307	1.00	19.87	A
	ATOM C	919	CG	ARG	A	232	187.205	153.647	10.172	1.00	20.99	A
45	ATOM C	920	CD	ARG	A	232	186.795	153.359	11.597	1.00	28.38	A
	ATOM N	921	NE	ARG	A	232	187.588	154.189	12.487	1.00	32.23	A
	ATOM C	922	CZ	ARG	A	232	188.247	153.745	13.545	1.00	31.41	A
50	ATOM N	923	NH1	ARG	A	232	188.213	152.459	13.873	1.00	29.13	A
	ATOM N	924	NH2	ARG	A	232	188.963	154.604	14.257	1.00	35.98	A
55	ATOM C	925	C	ARG	A	232	185.770	153.747	7.507	1.00	14.94	A
	ATOM O	926	O	ARG	A	232	185.356	154.866	7.761	1.00	12.98	A
60	ATOM N	927	N	THR	A	233	186.403	153.457	6.384	1.00	13.16	A
	ATOM C	928	CA	THR	A	233	186.652	154.446	5.361	1.00	13.60	A
	ATOM C	929	CB	THR	A	233	187.719	153.902	4.340	1.00	14.55	A

5	ATOM O	930	OG1	THR	A	233	188.937	153.623	5.048	1.00	14.87	A
	ATOM C	931	CG2	THR	A	233	188.016	154.908	3.231	1.00	13.20	A
	ATOM C	932	C	THR	A	233	185.339	154.863	4.686	1.00	13.47	A
	ATOM O	933	O	THR	A	233	185.090	156.056	4.508	1.00	12.81	A
10	ATOM N	934	N	ALA	A	234	184.481	153.901	4.353	1.00	11.54	A
	ATOM C	935	CA	ALA	A	234	183.199	154.225	3.713	1.00	12.90	A
15	ATOM C	936	CB	ALA	A	234	182.531	152.967	3.184	1.00	6.31	A
	ATOM C	937	C	ALA	A	234	182.254	154.953	4.675	1.00	15.13	A
20	ATOM O	938	O	ALA	A	234	181.498	155.843	4.272	1.00	18.25	A
	ATOM N	939	N	THR	A	235	182.297	154.579	5.945	1.00	13.08	A
	ATOM C	940	CA	THR	A	235	181.450	155.221	6.909	1.00	11.34	A
25	ATOM C	941	CB	THR	A	235	181.581	154.543	8.289	1.00	13.04	A
	ATOM O	942	OG1	THR	A	235	181.181	153.167	8.177	1.00	13.03	A
30	ATOM C	943	CG2	THR	A	235	180.679	155.235	9.304	1.00	9.30	A
	ATOM C	944	C	THR	A	235	181.813	156.701	6.976	1.00	12.76	A
	ATOM O	945	O	THR	A	235	180.930	157.553	6.894	1.00	14.21	A
35	ATOM N	946	N	TYR	A	236	183.104	157.003	7.115	1.00	12.83	A
	ATOM C	947	CA	TYR	A	236	183.586	158.392	7.157	1.00	14.72	A
40	ATOM C	948	CB	TYR	A	236	185.096	158.451	7.371	1.00	16.17	A
	ATOM C	949	CG	TYR	A	236	185.572	158.175	8.772	1.00	16.12	A
	ATOM C	950	CD1	TYR	A	236	184.785	158.491	9.876	1.00	16.03	A
45	ATOM C	951	CE1	TYR	A	236	185.237	158.261	11.162	1.00	16.90	A
	ATOM C	952	CD2	TYR	A	236	186.830	157.626	8.993	1.00	13.79	A
50	ATOM C	953	CE2	TYR	A	236	187.290	157.397	10.266	1.00	15.98	A
	ATOM C	954	CZ	TYR	A	236	186.490	157.709	11.347	1.00	19.04	A
	ATOM O	955	OH	TYR	A	236	186.935	157.420	12.609	1.00	22.33	A
55	ATOM C	956	C	TYR	A	236	183.291	159.154	5.862	1.00	16.50	A
	ATOM O	957	O	TYR	A	236	182.873	160.311	5.898	1.00	15.39	A
60	ATOM N	958	N	ILE	A	237	183.536	158.517	4.718	1.00	14.99	A
	ATOM C	959	CA	ILE	A	237	183.274	159.176	3.456	1.00	15.34	A
	ATOM C	960	CB	ILE	A	237	183.656	158.295	2.242	1.00	15.72	A

5	ATOM C	961	CG2	ILE	A	237	183.331	159.027	0.960	1.00	17.81	A
	ATOM C	962	CG1	ILE	A	237	185.157	157.993	2.241	1.00	13.11	A
	ATOM C	963	CD1	ILE	A	237	186.062	159.254	2.278	1.00	13.67	A
	ATOM C	964	C	ILE	A	237	181.795	159.542	3.379	1.00	17.56	A
10	ATOM O	965	O	ILE	A	237	181.442	160.638	2.953	1.00	18.55	A
	ATOM N	966	N	THR	A	238	180.935	158.626	3.804	1.00	17.36	A
15	ATOM C	967	CA	THR	A	238	179.489	158.853	3.816	1.00	14.99	A
	ATOM C	968	CB	THR	A	238	178.760	157.600	4.330	1.00	13.08	A
20	ATOM O	969	OG1	THR	A	238	179.059	156.502	3.464	1.00	16.26	A
	ATOM C	970	CG2	THR	A	238	177.257	157.817	4.354	1.00	13.58	A
	ATOM C	971	C	THR	A	238	179.069	160.037	4.696	1.00	14.23	A
	ATOM O	972	O	THR	A	238	178.214	160.829	4.307	1.00	14.27	A
25	ATOM N	973	N	GLU	A	239	179.649	160.149	5.888	1.00	11.63	A
	ATOM C	974	CA	GLU	A	239	179.285	161.242	6.781	1.00	13.23	A
30	ATOM C	975	CB	GLU	A	239	179.913	161.025	8.170	1.00	14.00	A
	ATOM C	976	CG	GLU	A	239	179.443	159.721	8.804	1.00	18.38	A
35	ATOM C	977	CD	GLU	A	239	180.121	159.365	10.124	1.00	24.00	A
	ATOM O	978	OE1	GLU	A	239	181.366	159.259	10.187	1.00	24.67	A
	ATOM O	979	OE2	GLU	A	239	179.385	159.158	11.114	1.00	32.52	A
	ATOM C	980	C	GLU	A	239	179.767	162.548	6.149	1.00	13.27	A
40	ATOM O	981	O	GLU	A	239	179.028	163.525	6.073	1.00	12.45	A
	ATOM N	982	N	LEU	A	240	181.005	162.538	5.668	1.00	11.05	A
45	ATOM C	983	CA	LEU	A	240	181.566	163.707	5.049	1.00	13.29	A
	ATOM C	984	CB	LEU	A	240	183.043	163.465	4.738	1.00	15.79	A
50	ATOM C	985	CG	LEU	A	240	183.894	164.638	4.235	1.00	16.19	A
	ATOM C	986	CD1	LEU	A	240	184.031	165.720	5.279	1.00	19.17	A
55	ATOM C	987	CD2	LEU	A	240	185.267	164.108	3.884	1.00	19.04	A
	ATOM C	988	C	LEU	A	240	180.798	164.081	3.773	1.00	13.39	A
60	ATOM O	989	O	LEU	A	240	180.513	165.256	3.548	1.00	14.19	A
	ATOM N	990	N	ALA	A	241	180.443	163.091	2.955	1.00	11.67	A
	ATOM C	991	CA	ALA	A	241	179.726	163.372	1.711	1.00	12.50	A

5	ATOM C	992	CB	ALA	A	241	179.577	162.108	0.873	1.00	9.22	A
	ATOM C	993	C	ALA	A	241	178.367	164.004	1.979	1.00	14.45	A
	ATOM O	994	O	ALA	A	241	177.923	164.878	1.222	1.00	14.36	A
	ATOM N	995	N	ASN	A	242	177.714	163.562	3.053	1.00	14.82	A
	ATOM C	996	CA	ASN	A	242	176.420	164.109	3.447	1.00	16.37	A
10	ATOM C	997	CB	ASN	A	242	175.822	163.329	4.619	1.00	20.05	A
	ATOM C	998	CG	ASN	A	242	175.213	162.005	4.210	1.00	22.16	A
15	ATOM O	999	OD1	ASN	A	242	175.027	161.133	5.055	1.00	23.63	A
	ATOM N	1000	ND2	ASN	A	242	174.883	161.850	2.922	1.00	24.84	A
20	ATOM C	1001	C	ASN	A	242	176.623	165.540	3.918	1.00	16.87	A
	ATOM O	1002	O	ASN	A	242	175.804	166.429	3.636	1.00	13.50	A
25	ATOM N	1003	N	ALA	A	243	177.713	165.747	4.656	1.00	13.07	A
	ATOM C	1004	CA	ALA	A	243	178.019	167.065	5.190	1.00	13.28	A
30	ATOM C	1005	CB	ALA	A	243	179.204	166.982	6.137	1.00	13.95	A
	ATOM C	1006	C	ALA	A	243	178.292	168.063	4.072	1.00	14.76	A
35	ATOM O	1007	O	ALA	A	243	177.751	169.173	4.080	1.00	11.54	A
	ATOM N	1008	N	LEU	A	244	179.126	167.651	3.113	1.00	15.34	A
40	ATOM C	1009	CA	LEU	A	244	179.487	168.477	1.955	1.00	14.00	A
	ATOM C	1010	CB	LEU	A	244	180.572	167.766	1.134	1.00	12.82	A
45	ATOM C	1011	CG	LEU	A	244	181.958	167.607	1.791	1.00	13.66	A
	ATOM C	1012	CD1	LEU	A	244	182.862	166.784	0.883	1.00	10.60	A
50	ATOM C	1013	CD2	LEU	A	244	182.570	168.990	2.068	1.00	10.59	A
	ATOM C	1014	C	LEU	A	244	178.245	168.764	1.078	1.00	13.84	A
55	ATOM O	1015	O	LEU	A	244	178.079	169.862	0.545	1.00	9.94	A
	ATOM N	1016	N	SER	A	245	177.363	167.776	0.949	1.00	11.65	A
60	ATOM C	1017	CA	SER	A	245	176.162	167.951	0.149	1.00	12.45	A
	ATOM C	1018	CB	SER	A	245	175.403	166.623	0.101	1.00	11.63	A
65	ATOM O	1019	OG	SER	A	245	174.265	166.724	-0.729	1.00	18.58	A
	ATOM C	1020	C	SER	A	245	175.284	169.090	0.716	1.00	12.58	A
70	ATOM O	1021	O	SER	A	245	174.753	169.925	-0.028	1.00	13.38	A
	ATOM N	1022	N	TYR	A	246	175.156	169.126	2.038	1.00	10.82	A

5	ATOM C	1023	CA	TYR	A	246	174.388	170.146	2.719	1.00	12.87	A
	ATOM C	1024	CB	TYR	A	246	174.337	169.838	4.232	1.00	10.92	A
	ATOM C	1025	CG	TYR	A	246	173.941	171.010	5.076	1.00	13.12	A
	ATOM C	1026	CD1	TYR	A	246	172.615	171.398	5.169	1.00	11.79	A
10	ATOM C	1027	CE1	TYR	A	246	172.249	172.526	5.886	1.00	15.75	A
	ATOM C	1028	CD2	TYR	A	246	174.905	171.782	5.727	1.00	14.34	A
	ATOM C	1029	CE2	TYR	A	246	174.548	172.925	6.452	1.00	17.65	A
15	ATOM C	1030	CZ	TYR	A	246	173.209	173.288	6.526	1.00	18.09	A
	ATOM O	1031	OH	TYR	A	246	172.806	174.411	7.231	1.00	20.69	A
20	ATOM C	1032	C	TYR	A	246	175.068	171.506	2.474	1.00	14.69	A
	ATOM O	1033	O	TYR	A	246	174.399	172.522	2.263	1.00	16.54	A
25	ATOM N	1034	N	CYS	A	247	176.398	171.506	2.526	1.00	12.79	A
	ATOM C	1035	CA	CYS	A	247	177.217	172.695	2.312	1.00	15.14	A
	ATOM C	1036	CB	CYS	A	247	178.697	172.339	2.453	1.00	18.30	A
30	ATOM S	1037	SG	CYS	A	247	179.389	172.397	4.097	1.00	20.02	A
	ATOM C	1038	C	CYS	A	247	177.033	173.298	0.930	1.00	14.64	A
35	ATOM O	1039	O	CYS	A	247	176.944	174.517	0.765	1.00	13.32	A
	ATOM N	1040	N	HIS	A	248	177.018	172.424	-0.063	1.00	12.96	A
	ATOM C	1041	CA	HIS	A	248	176.867	172.853	-1.435	1.00	14.92	A
40	ATOM C	1042	CB	HIS	A	248	177.246	171.711	-2.361	1.00	14.58	A
	ATOM C	1043	CG	HIS	A	248	178.698	171.388	-2.305	1.00	15.75	A
45	ATOM C	1044	CD2	HIS	A	248	179.651	171.777	-1.427	1.00	14.69	A
	ATOM N	1045	ND1	HIS	A	248	179.331	170.596	-3.236	1.00	18.18	A
	ATOM C	1046	CE1	HIS	A	248	180.614	170.512	-2.934	1.00	15.22	A
50	ATOM N	1047	NE2	HIS	A	248	180.832	171.220	-1.840	1.00	14.77	A
	ATOM C	1048	C	HIS	A	248	175.474	173.338	-1.717	1.00	16.00	A
55	ATOM O	1049	O	HIS	A	248	175.285	174.228	-2.538	1.00	16.44	A
	ATOM N	1050	N	SER	A	249	174.503	172.744	-1.028	1.00	14.49	A
	ATOM C	1051	CA	SER	A	249	173.125	173.148	-1.197	1.00	15.32	A
60	ATOM C	1052	CB	SER	A	249	172.201	172.233	-0.392	1.00	11.40	A
	ATOM O	1053	OG	SER	A	249	172.281	172.527	0.985	1.00	16.48	A

	5	ATOM C	1054	C	SER A 249	173.055	174.597	-0.696	1.00	16.09	A
		ATOM O	1055	O	SER A 249	172.139	175.350	-1.034	1.00	18.04	A
		ATOM N	1056	N	LYS A 250	174.031	174.988	0.118	1.00	15.99	A
		ATOM C	1057	CA	LYS A 250	174.072	176.363	0.599	1.00	15.13	A
	10	ATOM C	1058	CB	LYS A 250	174.405	176.441	2.107	1.00	13.57	A
		ATOM C	1059	CG	LYS A 250	173.350	175.850	3.040	1.00	15.19	A
		ATOM C	1060	CD	LYS A 250	171.930	176.203	2.629	1.00	19.05	A
	15	ATOM C	1061	CE	LYS A 250	170.943	175.150	3.131	1.00	24.43	A
		ATOM N	1062	NZ	LYS A 250	169.492	175.372	2.776	1.00	28.76	A
	20	ATOM C	1063	C	LYS A 250	175.106	177.133	-0.210	1.00	11.97	A
		ATOM O	1064	O	LYS A 250	175.375	178.286	0.957	1.00	14.99	A
		ATOM N	1065	N	ARG A 251	175.686	176.478	-1.208	1.00	14.14	A
	25	ATOM C	1066	CA	ARG A 251	176.690	177.099	-2.079	1.00	13.45	A
		ATOM C	1067	CB	ARG A 251	176.080	178.305	-2.792	1.00	14.05	A
		ATOM C	1068	CG	ARG A 251	174.976	177.936	-3.779	1.00	21.06	A
	30	ATOM C	1069	CD	ARG A 251	175.441	178.112	-5.227	1.00	27.95	A
		ATOM N	1070	NE	ARG A 251	175.547	176.844	-5.943	1.00	31.22	A
	35	ATOM C	1071	CZ	ARG A 251	176.391	176.615	-6.949	1.00	31.35	A
		ATOM N	1072	NH1	ARG A 251	177.214	177.570	-7.368	1.00	28.63	A
	40	ATOM N	1073	NH2	ARG A 251	176.427	175.422	-7.526	1.00	31.96	A
		ATOM C	1074	C	ARG A 251	177.974	177.493	-1.362	1.00	12.30	A
		ATOM O	1075	O	ARG A 251	178.618	178.472	-1.703	1.00	12.69	A
	45	ATOM N	1076	N	VAL A 252	178.344	176.714	-0.363	1.00	11.12	A
		ATOM C	1077	CA	VAL A 252	179.569	176.971	0.368	1.00	12.45	A
	50	ATOM C	1078	CB	VAL A 252	179.338	176.810	1.885	1.00	12.23	A
		ATOM C	1079	CG1	VAL A 252	180.651	176.509	2.587	1.00	9.08	A
		ATOM C	1080	CG2	VAL A 252	178.681	178.059	2.446	1.00	10.54	A
	55	ATOM C	1081	C	VAL A 252	180.604	175.940	-0.083	1.00	15.27	A
		ATOM O	1082	O	VAL A 252	180.267	174.774	-0.265	1.00	12.78	A
	60	ATOM N	1083	N	ILE A 253	181.840	176.373	-0.326	1.00	13.72	A
		ATOM C	1084	CA	ILE A 253	182.872	175.419	-0.680	1.00	10.89	A

5	ATOM C	1085	CB	ILE	A	253	183.670	175.788	-1.957	1.00	11.67	A
	ATOM C	1086	CG2	ILE	A	253	184.426	174.535	-2.441	1.00	5.83	A
	ATOM C	1087	CG1	ILE	A	253	182.733	176.323	-3.059	1.00	10.28	A
	ATOM C	1088	CD1	ILE	A	253	183.439	176.812	-4.329	1.00	3.57	A
10	ATOM C	1089	C	ILE	A	253	183.831	175.453	0.498	1.00	13.01	A
	ATOM O	1090	O	ILE	A	253	184.347	176.524	0.849	1.00	13.11	A
15	ATOM N	1091	N	HIS	A	254	184.050	174.288	1.113	1.00	13.19	A
	ATOM C	1092	CA	HIS	A	254	184.943	174.161	2.259	1.00	12.95	A
20	ATOM C	1093	CB	HIS	A	254	184.868	172.745	2.843	1.00	12.70	A
	ATOM C	1094	CG	HIS	A	254	185.587	172.606	4.160	1.00	12.92	A
	ATOM C	1095	CD2	HIS	A	254	185.206	172.914	5.423	1.00	9.91	A
	ATOM N	1096	ND1	HIS	A	254	186.898	172.180	4.257	1.00	13.73	A
25	ATOM C	1097	CE1	HIS	A	254	187.290	172.229	5.515	1.00	10.14	A
	ATOM N	1098	NE2	HIS	A	254	186.282	172.671	6.243	1.00	11.29	A
30	ATOM C	1099	C	HIS	A	254	186.383	174.507	1.889	1.00	13.04	A
	ATOM O	1100	O	HIS	A	254	186.971	175.438	2.447	1.00	14.41	A
35	ATOM N	1101	N	ARG	A	255	186.935	173.743	0.953	1.00	12.07	A
	ATOM C	1102	CA	ARG	A	255	188.291	173.910	0.438	1.00	12.35	A
	ATOM C	1103	CB	ARG	A	255	188.494	175.341	-0.050	1.00	13.05	A
40	ATOM C	1104	CG	ARG	A	255	187.553	175.664	-1.200	1.00	15.96	A
	ATOM C	1105	CD	ARG	A	255	187.942	176.885	-1.997	1.00	11.42	A
45	ATOM N	1106	NE	ARG	A	255	188.045	178.075	-1.183	1.00	13.42	A
	ATOM C	1107	CZ	ARG	A	255	188.194	179.295	-1.690	1.00	17.97	A
	ATOM N	1108	NH1	ARG	A	255	188.248	179.453	-3.012	1.00	12.59	A
50	ATOM N	1109	NH2	ARG	A	255	188.308	180.348	-0.880	1.00	11.08	A
	ATOM C	1110	C	ARG	A	255	189.479	173.491	1.328	1.00	14.82	A
55	ATOM O	1111	O	ARG	A	255	190.628	173.656	0.914	1.00	16.45	A
	ATOM N	1112	N	ASP	A	256	189.237	172.959	2.528	1.00	13.90	A
60	ATOM C	1113	CA	ASP	A	256	190.355	172.522	3.364	1.00	14.13	A
	ATOM C	1114	CB	ASP	A	256	190.779	173.631	4.341	1.00	15.61	A
	ATOM C	1115	CG	ASP	A	256	192.185	173.408	4.930	1.00	17.71	A

5	ATOM O	1116	OD1	ASP	A	256	193.119	172.950	4.217	1.00	18.23	A
	ATOM O	1117	OD2	ASP	A	256	192.364	173.712	6.130	1.00	20.01	A
	ATOM C	1118	C	ASP	A	256	190.021	171.231	4.094	1.00	14.83	A
	ATOM O	1119	O	ASP	A	256	190.209	171.088	5.300	1.00	17.90	A
10	ATOM N	1120	N	ILE	A	257	189.522	170.285	3.321	1.00	14.83	A
	ATOM C	1121	CA	ILE	A	257	189.170	168.978	3.809	1.00	15.89	A
15	ATOM C	1122	CB	ILE	A	257	188.209	168.318	2.821	1.00	16.68	A
	ATOM C	1123	CG2	ILE	A	257	188.096	166.834	3.106	1.00	18.21	A
20	ATOM C	1124	CG1	ILE	A	257	186.851	169.010	2.909	1.00	19.11	A
	ATOM C	1125	CD1	ILE	A	257	185.939	168.636	1.771	1.00	26.98	A
	ATOM C	1126	C	ILE	A	257	190.461	168.170	3.888	1.00	16.84	A
	ATOM O	1127	O	ILE	A	257	191.180	168.019	2.890	1.00	19.23	A
25	ATOM N	1128	N	LYS	A	258	190.759	167.673	5.079	1.00	14.42	A
	ATOM C	1129	CA	LYS	A	258	191.948	166.861	5.321	1.00	13.61	A
30	ATOM C	1130	CB	LYS	A	258	193.218	167.696	5.165	1.00	11.12	A
	ATOM C	1131	CG	LYS	A	258	193.288	168.912	6.021	1.00	10.35	A
35	ATOM C	1132	CD	LYS	A	258	194.685	169.397	5.941	1.00	11.98	A
	ATOM C	1133	CE	LYS	A	258	194.946	170.539	6.844	1.00	10.31	A
	ATOM N	1134	NZ	LYS	A	258	196.316	171.028	6.523	1.00	13.12	A
	ATOM C	1135	C	LYS	A	258	191.828	166.275	6.728	1.00	12.82	A
40	ATOM O	1136	O	LYS	A	258	191.093	166.807	7.565	1.00	12.94	A
	ATOM N	1137	N	PRO	A	259	192.547	165.180	7.011	1.00	13.48	A
45	ATOM C	1138	CD	PRO	A	259	193.607	164.582	6.181	1.00	11.93	A
	ATOM C	1139	CA	PRO	A	259	192.487	164.525	8.329	1.00	14.07	A
50	ATOM C	1140	CB	PRO	A	259	193.641	163.517	8.267	1.00	14.89	A
	ATOM C	1141	CG	PRO	A	259	193.714	163.197	6.778	1.00	14.98	A
55	ATOM C	1142	C	PRO	A	259	192.527	165.413	9.583	1.00	15.36	A
	ATOM O	1143	O	PRO	A	259	191.773	165.171	10.520	1.00	15.88	A
	ATOM N	1144	N	GLU	A	260	193.388	166.428	9.593	1.00	15.22	A
60	ATOM C	1145	CA	GLU	A	260	193.516	167.340	10.734	1.00	19.96	A
	ATOM C	1146	CB	GLU	A	260	194.770	168.225	10.563	1.00	22.41	A

5	ATOM C	1147	CG	GLU	A	260	196.090	167.457	10.516	1.00	29.11	A
	ATOM C	1148	CD	GLU	A	260	196.610	167.140	9.092	1.00	32.88	A
	ATOM O	1149	OE1	GLU	A	260	195.826	166.656	8.235	1.00	33.12	A
	ATOM O	1150	OE2	GLU	A	260	197.823	167.360	8.841	1.00	35.49	A
10	ATOM C	1151	C	GLU	A	260	192.280	168.252	10.924	1.00	18.80	A
	ATOM O	1152	O	GLU	A	260	192.140	168.905	11.957	1.00	18.71	A
15	ATOM N	1153	N	ASN	A	261	191.401	168.309	9.922	1.00	16.14	A
	ATOM C	1154	CA	ASN	A	261	190.206	169.139	10.014	1.00	14.12	A
	ATOM C	1155	CB	ASN	A	261	190.084	170.036	8.799	1.00	12.74	A
20	ATOM C	1156	CG	ASN	A	261	191.068	171.176	8.824	1.00	12.37	A
	ATOM O	1157	OD1	ASN	A	261	191.719	171.446	9.840	1.00	11.65	A
25	ATOM N	1158	ND2	ASN	A	261	191.178	171.868	7.705	1.00	11.18	A
	ATOM C	1159	C	ASN	A	261	188.944	168.329	10.159	1.00	14.87	A
	ATOM O	1160	O	ASN	A	261	187.844	168.855	10.027	1.00	14.12	A
30	ATOM N	1161	N	LEU	A	262	189.117	167.037	10.428	1.00	16.20	A
	ATOM C	1162	CA	LEU	A	262	187.996	166.127	10.596	1.00	13.58	A
35	ATOM C	1163	CB	LEU	A	262	188.128	164.954	9.627	1.00	13.22	A
	ATOM C	1164	CG	LEU	A	262	188.164	165.406	8.162	1.00	15.01	A
	ATOM C	1165	CD1	LEU	A	262	188.502	164.230	7.232	1.00	8.10	A
40	ATOM C	1166	CD2	LEU	A	262	186.807	166.049	7.834	1.00	10.56	A
	ATOM C	1167	C	LEU	A	262	188.027	165.633	12.031	1.00	15.43	A
45	ATOM O	1168	O	LEU	A	262	188.999	165.008	12.459	1.00	17.59	A
	ATOM N	1169	N	LEU	A	263	186.968	165.915	12.777	1.00	11.89	A
	ATOM C	1170	CA	LEU	A	263	186.926	165.505	14.154	1.00	10.46	A
50	ATOM C	1171	CB	LEU	A	263	186.657	166.725	15.005	1.00	13.46	A
	ATOM C	1172	CG	LEU	A	263	187.584	167.921	14.699	1.00	14.28	A
55	ATOM C	1173	CD1	LEU	A	263	187.208	169.055	15.634	1.00	15.02	A
	ATOM C	1174	CD2	LEU	A	263	189.050	167.563	14.865	1.00	12.28	A
	ATOM C	1175	C	LEU	A	263	185.905	164.407	14.409	1.00	12.75	A
60	ATOM O	1176	O	LEU	A	263	185.068	164.112	13.553	1.00	13.83	A
	ATOM N	1177	N	LEU	A	264	185.989	163.780	15.576	1.00	13.44	A

5	ATOM C	1178	CA	LEU	A	264	185.076	162.693	15.919	1.00	15.08	A
	ATOM C	1179	CB	LEU	A	264	185.856	161.421	16.298	1.00	15.27	A
	ATOM C	1180	CG	LEU	A	264	186.808	160.821	15.263	1.00	16.94	A
	ATOM C	1181	CD1	LEU	A	264	187.393	159.499	15.783	1.00	20.04	A
10	ATOM C	1182	CD2	LEU	A	264	186.043	160.590	13.944	1.00	16.69	A
	ATOM C	1183	C	LEU	A	264	184.190	163.103	17.078	1.00	14.83	A
	ATOM O	1184	O	LEU	A	264	184.669	163.613	18.096	1.00	13.07	A
15	ATOM N	1185	N	GLY	A	265	182.890	162.881	16.907	1.00	14.85	A
	ATOM C	1186	CA	GLY	A	265	181.943	163.218	17.947	1.00	15.69	A
20	ATOM C	1187	C	GLY	A	265	181.844	162.127	18.999	1.00	17.48	A
	ATOM O	1188	O	GLY	A	265	182.597	161.144	18.989	1.00	19.40	A
	ATOM N	1189	N	SER	A	266	180.888	162.306	19.899	1.00	17.64	A
25	ATOM C	1190	CA	SER	A	266	180.641	161.398	21.007	1.00	18.83	A
	ATOM C	1191	CB	SER	A	266	179.417	161.895	21.766	1.00	17.49	A
30	ATOM O	1192	OG	SER	A	266	179.347	161.294	23.037	1.00	31.06	A
	ATOM C	1193	C	SER	A	266	180.457	159.923	20.615	1.00	16.59	A
	ATOM O	1194	O	SER	A	266	180.771	159.025	21.389	1.00	16.64	A
35	ATOM N	1195	N	ALA	A	267	179.960	159.675	19.412	1.00	15.97	A
	ATOM C	1196	CA	ALA	A	267	179.731	158.314	18.939	1.00	17.67	A
40	ATOM C	1197	CB	ALA	A	267	178.288	158.163	18.456	1.00	14.65	A
	ATOM C	1198	C	ALA	A	267	180.670	157.930	17.815	1.00	18.92	A
	ATOM O	1199	O	ALA	A	267	180.353	157.040	17.025	1.00	21.00	A
45	ATOM N	1200	N	GLY	A	268	181.812	158.604	17.716	1.00	21.24	A
	ATOM C	1201	CA	GLY	A	268	182.741	158.278	16.648	1.00	22.38	A
50	ATOM C	1202	C	GLY	A	268	182.289	158.773	15.282	1.00	21.15	A
	ATOM O	1203	O	GLY	A	268	182.809	158.323	14.266	1.00	20.78	A
	ATOM N	1204	N	GLU	A	269	181.324	159.690	15.249	1.00	19.71	A
55	ATOM C	1205	CA	GLU	A	269	180.831	160.239	13.983	1.00	18.83	A
	ATOM C	1206	CB	GLU	A	269	179.386	160.746	14.107	1.00	20.11	A
60	ATOM C	1207	CG	GLU	A	269	179.239	162.020	14.944	1.00	27.28	A
	ATOM C	1208	CD	GLU	A	269	178.874	161.722	16.385	1.00	29.04	A

5	ATOM O	1209	OE1	GLU	A	269	179.762	161.324	17.177	1.00	30.97	A
	ATOM O	1210	OE2	GLU	A	269	177.677	161.868	16.711	1.00	33.63	A
	ATOM C	1211	C	GLU	A	269	181.702	161.409	13.549	1.00	17.27	A
	ATOM O	1212	O	GLU	A	269	182.088	162.249	14.368	1.00	15.38	A
10	ATOM N	1213	N	LEU	A	270	181.994	161.461	12.253	1.00	14.97	A
	ATOM C	1214	CA	LEU	A	270	182.822	162.515	11.689	1.00	15.39	A
15	ATOM C	1215	CB	LEU	A	270	183.169	162.167	10.229	1.00	21.78	A
	ATOM C	1216	CG	LEU	A	270	184.100	163.071	9.408	1.00	22.18	A
	ATOM C	1217	CD1	LEU	A	270	185.484	162.839	9.938	1.00	26.73	A
20	ATOM C	1218	CD2	LEU	A	270	184.109	162.725	7.944	1.00	27.39	A
	ATOM C	1219	C	LEU	A	270	182.129	163.876	11.722	1.00	13.13	A
25	ATOM O	1220	O	LEU	A	270	180.932	163.973	11.490	1.00	12.45	A
	ATOM N	1221	N	LYS	A	271	182.895	164.918	12.027	1.00	13.69	A
	ATOM C	1222	CA	LYS	A	271	182.395	166.296	12.025	1.00	13.80	A
30	ATOM C	1223	CB	LYS	A	271	182.201	166.814	13.450	1.00	13.22	A
	ATOM C	1224	CG	LYS	A	271	180.846	166.378	14.025	1.00	16.86	A
35	ATOM C	1225	CD	LYS	A	271	180.790	166.428	15.509	1.00	17.04	A
	ATOM C	1226	CE	LYS	A	271	179.494	165.823	15.967	1.00	15.79	A
	ATOM N	1227	NZ	LYS	A	271	178.379	166.692	15.545	1.00	20.81	A
40	ATOM C	1228	C	LYS	A	271	183.392	167.151	11.270	1.00	15.22	A
	ATOM O	1229	O	LYS	A	271	184.586	167.152	11.582	1.00	16.95	A
45	ATOM N	1230	N	ILE	A	272	182.919	167.842	10.238	1.00	15.55	A
	ATOM C	1231	CA	ILE	A	272	183.803	168.702	9.462	1.00	15.61	A
	ATOM C	1232	CB	ILE	A	272	183.143	169.220	8.163	1.00	19.61	A
50	ATOM C	1233	CG2	ILE	A	272	184.054	170.269	7.530	1.00	18.20	A
	ATOM C	1234	CG1	ILE	A	272	182.850	168.069	7.203	1.00	22.81	A
55	ATOM C	1235	CD1	ILE	A	272	182.068	168.504	5.967	1.00	25.62	A
	ATOM C	1236	C	ILE	A	272	184.051	169.926	10.303	1.00	13.27	A
	ATOM O	1237	O	ILE	A	272	183.136	170.422	10.945	1.00	12.04	A
60	ATOM N	1238	N	ALA	A	273	185.270	170.428	10.294	1.00	11.17	A
	ATOM C	1239	CA	ALA	A	273	185.568	171.623	11.069	1.00	13.73	A

5	ATOM C	1240	CB	ALA A 273	186.266	171.248	12.376	1.00	10.14	A
	ATOM C	1241	C	ALA A 273	186.472	172.498	10.225	1.00	16.38	A
	ATOM O	1242	O	ALA A 273	186.688	172.208	9.047	1.00	16.96	A
	ATOM N	1243	N	ASP A 274	186.986	173.568	10.834	1.00	17.04	A
	ATOM C	1244	CA	ASP A 274	187.913	174.500	10.200	1.00	15.18	A
10	ATOM C	1245	CB	ASP A 274	189.288	173.805	10.074	1.00	17.02	A
	ATOM C	1246	CG	ASP A 274	190.447	174.786	9.800	1.00	19.27	A
	ATOM O	1247	OD1	ASP A 274	190.190	175.999	9.635	1.00	22.45	A
15	ATOM O	1248	OD2	ASP A 274	191.624	174.338	9.753	1.00	17.87	A
	ATOM C	1249	C	ASP A 274	187.434	175.064	8.838	1.00	16.14	A
	ATOM O	1250	O	ASP A 274	187.846	174.604	7.776	1.00	12.68	A
20	ATOM N	1251	N	PHE A 275	186.559	176.065	8.881	1.00	15.86	A
	ATOM C	1252	CA	PHE A 275	186.074	176.688	7.666	1.00	14.12	A
	ATOM C	1253	CB	PHE A 275	184.602	177.108	7.835	1.00	13.16	A
25	ATOM C	1254	CG	PHE A 275	183.640	175.948	7.721	1.00	12.72	A
	ATOM C	1255	CD1	PHE A 275	183.540	174.994	8.746	1.00	11.42	A
	ATOM C	1256	CD2	PHE A 275	182.936	175.727	6.535	1.00	11.44	A
30	ATOM C	1257	CE1	PHE A 275	182.768	173.843	8.581	1.00	10.04	A
	ATOM C	1258	CE2	PHE A 275	182.157	174.568	6.367	1.00	12.57	A
	ATOM C	1259	CZ	PHE A 275	182.079	173.631	7.396	1.00	11.15	A
35	ATOM C	1260	C	PHE A 275	186.966	177.868	7.289	1.00	15.87	A
	ATOM O	1261	O	PHE A 275	186.541	178.780	6.568	1.00	15.07	A
	ATOM N	1262	N	GLY A 276	188.221	177.820	7.751	1.00	15.09	A
40	ATOM C	1263	CA	GLY A 276	189.184	178.875	7.452	1.00	17.20	A
	ATOM C	1264	C	GLY A 276	189.322	179.285	5.983	1.00	16.44	A
	ATOM O	1265	O	GLY A 276	189.368	180.482	5.665	1.00	17.13	A
45	ATOM N	1266	N	TRP A 277	189.378	178.307	5.082	1.00	13.73	A
	ATOM C	1267	CA	TRP A 277	189.514	178.596	3.664	1.00	14.40	A
	ATOM C	1268	CB	TRP A 277	190.568	177.667	3.071	1.00	20.13	A
50	ATOM C	1269	CG	TRP A 277	191.860	177.753	3.789	1.00	22.40	A
	ATOM C	1270	CD2	TRP A 277	192.691	178.904	3.893	1.00	23.73	A

5	ATOM C	1271	CE2	TRP	A	277	193.788	178.558	4.701	1.00	26.05	A
	ATOM C	1272	CE3	TRP	A	277	192.617	180.198	3.375	1.00	25.94	A
	ATOM C	1273	CD1	TRP	A	277	192.463	176.777	4.517	1.00	23.25	A
	ATOM N	1274	NE1	TRP	A	277	193.625	177.250	5.074	1.00	24.53	A
10	ATOM C	1275	CZ2	TRP	A	277	194.806	179.467	5.015	1.00	27.86	A
	ATOM C	1276	CZ3	TRP	A	277	193.631	181.106	3.686	1.00	28.74	A
	ATOM C	1277	CH2	TRP	A	277	194.711	180.733	4.496	1.00	26.68	A
15	ATOM C	1278	C	TRP	A	277	188.202	178.467	2.888	1.00	13.46	A
	ATOM O	1279	O	TRP	A	277	188.190	178.362	1.664	1.00	14.44	A
20	ATOM N	1280	N	SER	A	278	187.097	178.481	3.605	1.00	14.67	A
	ATOM C	1281	CA	SER	A	278	185.809	178.360	2.973	1.00	16.81	A
25	ATOM C	1282	CB	SER	A	278	184.785	177.937	4.009	1.00	18.65	A
	ATOM O	1283	OG	SER	A	278	185.042	176.588	4.334	1.00	31.56	A
	ATOM C	1284	C	SER	A	278	185.338	179.620	2.269	1.00	15.59	A
30	ATOM O	1285	O	SER	A	278	185.887	180.700	2.456	1.00	13.40	A
	ATOM N	1286	N	VAL	A	279	184.330	179.468	1.427	1.00	12.47	A
35	ATOM C	1287	CA	VAL	A	279	183.790	180.622	0.750	1.00	15.04	A
	ATOM C	1288	CB	VAL	A	279	184.631	181.010	-0.524	1.00	14.76	A
	ATOM C	1289	CG1	VAL	A	279	184.436	179.985	-1.646	1.00	10.49	A
40	ATOM C	1290	CG2	VAL	A	279	184.256	182.419	-0.971	1.00	9.51	A
	ATOM C	1291	C	VAL	A	279	182.347	180.399	0.352	1.00	15.66	A
45	ATOM O	1292	O	VAL	A	279	181.902	179.259	0.162	1.00	16.74	A
	ATOM N	1293	N	HIS	A	280	181.604	181.491	0.276	1.00	14.84	A
	ATOM C	1294	CA	HIS	A	280	180.224	181.389	-0.133	1.00	17.48	A
50	ATOM C	1295	CB	HIS	A	280	179.332	182.330	0.694	1.00	14.36	A
	ATOM C	1296	CG	HIS	A	280	177.885	182.230	0.336	1.00	16.95	A
55	ATOM C	1297	CD2	HIS	A	280	177.154	181.176	-0.102	1.00	16.10	A
	ATOM N	1298	ND1	HIS	A	280	177.045	183.323	0.300	1.00	15.76	A
	ATOM C	1299	CE1	HIS	A	280	175.864	182.946	-0.154	1.00	17.22	A
60	ATOM N	1300	NE2	HIS	A	280	175.903	181.648	-0.407	1.00	18.56	A
	ATOM C	1301	C	HIS	A	280	180.236	181.772	-1.622	1.00	17.74	A

	ATOM											
	O	1302	O	HIS	A	280	180.439	182.942	-1.989	1.00	16.22	A
	N	1303	N	ALA	A	281	180.048	180.773	-2.480	1.00	15.79	A
5	C	1304	CA	ALA	A	281	180.066	180.984	-3.930	1.00	17.35	A
	C	1305	CB	ALA	A	281	181.103	180.047	-4.565	1.00	15.43	A
10	C	1306	C	ALA	A	281	178.693	180.779	-4.610	1.00	18.31	A
	O	1307	O	ALA	A	281	178.489	179.809	-5.311	1.00	18.09	A
	N	1308	N	PRO	A	282	177.754	181.726	-4.412	1.00	20.27	A
15	C	1309	CD	PRO	A	282	177.983	182.946	-3.597	1.00	20.44	A
	C	1310	CA	PRO	A	282	176.381	181.701	-4.974	1.00	21.92	A
20	C	1311	CB	PRO	A	282	175.770	183.032	-4.483	1.00	21.47	A
	C	1312	CG	PRO	A	282	176.575	183.413	-3.327	1.00	21.85	A
	C	1313	C	PRO	A	282	176.326	181.581	-6.480	1.00	22.24	A
25	O	1314	O	PRO	A	282	175.611	180.729	-6.987	1.00	24.89	A
	N	1315	N	SER	A	283	177.088	182.439	-7.163	1.00	24.90	A
30	C	1316	CA	SER	A	283	177.131	182.464	-8.629	1.00	28.30	A
	C	1317	CB	SER	A	283	176.711	183.837	-9.202	1.00	26.31	A
	O	1318	OG	SER	A	283	175.659	184.461	-8.492	1.00	30.72	A
35	C	1319	C	SER	A	283	178.454	182.133	-9.327	1.00	27.14	A
	O	1320	O	SER	A	283	178.563	181.133	-10.033	1.00	31.35	A
40	N	1321	N	SER	A	284	179.434	183.011	-9.147	1.00	25.92	A
	C	1322	CA	SER	A	284	180.749	182.937	-9.789	1.00	26.41	A
	C	1323	CB	SER	A	284	181.476	184.252	-9.583	1.00	26.11	A
45	O	1324	OG	SER	A	284	180.590	185.288	-9.231	1.00	32.06	A
	C	1325	C	SER	A	284	181.720	181.869	-9.346	1.00	24.70	A
50	O	1326	O	SER	A	284	181.617	181.347	-8.254	1.00	26.06	A
	N	1327	N	ARG	A	285	182.717	181.636	-10.192	1.00	23.60	A
	C	1328	CA	ARG	A	285	183.782	180.701	-9.910	1.00	25.00	A
55	C	1329	CB	ARG	A	285	184.337	180.169	-11.225	1.00	25.95	A
	C	1330	CG	ARG	A	285	183.367	179.201	-11.935	1.00	31.00	A
60	C	1331	CD	ARG	A	285	184.154	178.152	-12.746	1.00	38.12	A
	N	1332	NE	ARG	A	285	184.419	178.543	-14.135	1.00	42.96	A

5	ATOM C	1333	CZ	ARG	A	285	185.202	177.856	-14.971	1.00	45.91	A
	ATOM N	1334	NH1	ARG	A	285	185.808	176.744	-14.560	1.00	46.53	A
10	ATOM N	1335	NH2	ARG	A	285	185.364	178.267	-16.225	1.00	46.52	A
	ATOM C	1336	C	ARG	A	285	184.869	181.436	-9.074	1.00	23.19	A
15	ATOM O	1337	O	ARG	A	285	184.791	182.652	-8.873	1.00	23.63	A
	ATOM N	1338	N	ARG	A	286	185.871	180.720	-8.578	1.00	22.25	A
20	ATOM C	1339	CA	ARG	A	286	186.898	181.369	-7.770	1.00	18.11	A
	ATOM C	1340	CB	ARG	A	286	186.781	180.826	-6.344	1.00	16.41	A
25	ATOM C	1341	CG	ARG	A	286	185.467	181.252	-5.671	1.00	17.03	A
	ATOM C	1342	CD	ARG	A	286	185.642	182.655	-5.179	1.00	16.99	A
30	ATOM N	1343	NE	ARG	A	286	184.443	183.221	-4.632	1.00	25.38	A
	ATOM C	1344	CZ	ARG	A	286	184.398	184.417	-4.072	1.00	26.94	A
35	ATOM N	1345	NH1	ARG	A	286	185.509	185.138	-3.995	1.00	28.48	A
	ATOM N	1346	NH2	ARG	A	286	183.244	184.894	-3.605	1.00	30.62	A
40	ATOM C	1347	C	ARG	A	286	188.309	181.189	-8.339	1.00	19.47	A
	ATOM O	1348	O	ARG	A	286	188.537	180.305	-9.174	1.00	17.62	A
45	ATOM N	1349	N	TPO	A	287	189.226	182.041	-7.916	1.00	21.77	A
	ATOM C	1350	CA	TPO	A	287	190.558	181.974	-8.377	1.00	21.28	A
50	ATOM C	1351	CB	TPO	A	287	190.775	183.306	-9.113	1.00	25.22	A
	ATOM C	1352	CG2	TPO	A	287	189.942	183.372	-10.421	1.00	22.17	A
55	ATOM O	1353	OG1	TPO	A	287	190.484	184.557	-8.448	1.00	33.29	A
	ATOM P	1354	P	TPO	A	287	191.582	185.763	-8.444	1.00	33.70	A
60	ATOM O	1355	O1P	TPO	A	287	190.902	186.991	-9.195	1.00	41.17	A
	ATOM O	1356	O2P	TPO	A	287	192.847	185.199	-9.239	1.00	37.62	A
65	ATOM O	1357	O3P	TPO	A	287	191.990	186.067	-6.912	1.00	41.70	A
	ATOM C	1358	C	TPO	A	287	191.612	181.717	-7.265	1.00	16.99	A
70	ATOM O	1359	O	TPO	A	287	192.886	181.536	-7.600	1.00	25.86	A
	ATOM N	1360	N	TPO	A	288	191.139	181.614	-6.033	1.00	16.91	A
75	ATOM C	1361	CA	TPO	A	288	192.066	181.441	-4.938	1.00	16.31	A
	ATOM C	1362	CB	TPO	A	288	191.262	181.750	-3.672	1.00	18.77	A
80	ATOM C	1363	CG2	TPO	A	288	192.190	181.949	-2.512	1.00	16.50	A

5	ATOM O	1364	OG1	TPO	A	288	190.694	183.015	-3.936	1.00	23.64	A
	ATOM P	1365	P	TPO	A	288	189.163	183.188	-3.329	1.00	18.56	A
	ATOM O	1366	O1P	TPO	A	288	189.234	182.723	-1.818	1.00	19.25	A
	ATOM O	1367	O2P	TPO	A	288	188.217	182.242	-4.154	1.00	24.67	A
10	ATOM O	1368	O3P	TPO	A	288	188.820	184.760	-3.320	1.00	24.29	A
	ATOM C	1369	C	TPO	A	288	192.828	180.109	-4.873	1.00	17.62	A
15	ATOM O	1370	O	TPO	A	288	192.132	178.986	-5.036	1.00	16.48	A
	ATOM N	1371	N	LEU	A	289	194.152	180.122	-4.825	1.00	19.62	A
20	ATOM C	1372	CA	LEU	A	289	194.793	178.875	-4.419	1.00	20.29	A
	ATOM C	1373	CB	LEU	A	289	196.229	178.759	-4.993	1.00	21.71	A
	ATOM C	1374	CG	LEU	A	289	196.977	177.458	-4.598	1.00	25.59	A
	ATOM C	1375	CD1	LEU	A	289	196.506	176.298	-5.488	1.00	30.17	A
25	ATOM C	1376	CD2	LEU	A	289	198.475	177.596	-4.769	1.00	26.69	A
	ATOM C	1377	C	LEU	A	289	194.833	178.800	-2.900	1.00	17.60	A
30	ATOM O	1378	O	LEU	A	289	195.428	179.646	-2.272	1.00	20.61	A
	ATOM N	1379	N	CYS	A	290	194.191	177.810	-2.307	1.00	16.97	A
35	ATOM C	1380	CA	CYS	A	290	194.204	177.679	-0.844	1.00	18.91	A
	ATOM C	1381	CB	CYS	A	290	193.102	178.535	-0.201	1.00	16.86	A
	ATOM S	1382	SG	CYS	A	290	191.434	178.234	-0.820	1.00	22.10	A
40	ATOM C	1383	C	CYS	A	290	194.003	176.211	-0.453	1.00	17.81	A
	ATOM O	1384	O	CYS	A	290	193.554	175.403	-1.266	1.00	15.28	A
45	ATOM N	1385	N	GLY	A	291	194.340	175.862	0.786	1.00	19.11	A
	ATOM C	1386	CA	GLY	A	291	194.203	174.484	1.227	1.00	18.98	A
	ATOM C	1387	C	GLY	A	291	195.536	173.896	1.644	1.00	19.71	A
50	ATOM O	1388	O	GLY	A	291	196.458	174.606	2.047	1.00	21.01	A
	ATOM N	1389	N	THR	A	292	195.626	172.584	1.523	1.00	18.60	A
55	ATOM C	1390	CA	THR	A	292	196.800	171.837	1.903	1.00	16.87	A
	ATOM C	1391	CB	THR	A	292	196.378	170.657	2.760	1.00	19.75	A
	ATOM O	1392	OG1	THR	A	292	195.457	171.126	3.752	1.00	25.57	A
60	ATOM C	1393	CG2	THR	A	292	197.563	169.991	3.407	1.00	18.64	A
	ATOM C	1394	C	THR	A	292	197.453	171.308	0.652	1.00	17.38	A

5	ATOM O	1395	O	THR	A	292	196.772	170.864	-0.269	1.00	16.20	A
	ATOM N	1396	N	LEU	A	293	198.780	171.347	0.631	1.00	18.38	A
	ATOM C	1397	CA	LEU	A	293	199.545	170.868	-0.511	1.00	18.67	A
	ATOM C	1398	CB	LEU	A	293	201.011	170.747	-0.102	1.00	18.33	A
10	ATOM C	1399	CG	LEU	A	293	201.947	170.217	-1.188	1.00	19.70	A
	ATOM C	1400	CD1	LEU	A	293	201.997	171.229	-2.316	1.00	20.14	A
15	ATOM C	1401	CD2	LEU	A	293	203.332	169.962	-0.603	1.00	18.52	A
	ATOM C	1402	C	LEU	A	293	199.063	169.533	-1.126	1.00	19.06	A
	ATOM O	1403	O	LEU	A	293	198.654	169.496	-2.287	1.00	16.78	A
20	ATOM N	1404	N	ASP	A	294	199.106	168.447	-0.355	1.00	16.52	A
	ATOM C	1405	CA	ASP	A	294	198.701	167.143	-0.868	1.00	15.08	A
25	ATOM C	1406	CB	ASP	A	294	199.029	166.048	0.164	1.00	19.73	A
	ATOM C	1407	CG	ASP	A	294	200.527	165.669	0.175	1.00	23.92	A
	ATOM O	1408	OD1	ASP	A	294	201.065	165.254	-0.891	1.00	23.94	A
30	ATOM O	1409	OD2	ASP	A	294	201.161	165.783	1.245	1.00	24.71	A
	ATOM C	1410	C	ASP	A	294	197.239	167.026	-1.309	1.00	14.50	A
35	ATOM O	1411	O	ASP	A	294	196.875	166.084	-2.011	1.00	11.76	A
	ATOM N	1412	N	TYR	A	295	196.411	167.996	-0.923	1.00	13.78	A
	ATOM C	1413	CA	TYR	A	295	194.993	167.963	-1.267	1.00	12.35	A
40	ATOM C	1414	CB	TYR	A	295	194.156	168.157	-0.001	1.00	12.74	A
	ATOM C	1415	CG	TYR	A	295	194.061	166.933	0.868	1.00	16.79	A
45	ATOM C	1416	CD1	TYR	A	295	195.179	166.449	1.561	1.00	19.00	A
	ATOM C	1417	CE1	TYR	A	295	195.119	165.265	2.307	1.00	18.70	A
	ATOM C	1418	CD2	TYR	A	295	192.871	166.216	0.947	1.00	16.93	A
50	ATOM C	1419	CE2	TYR	A	295	192.792	165.035	1.682	1.00	21.69	A
	ATOM C	1420	CZ	TYR	A	295	193.916	164.559	2.357	1.00	22.19	A
55	ATOM O	1421	OH	TYR	A	295	193.805	163.362	3.046	1.00	26.24	A
	ATOM C	1422	C	TYR	A	295	194.542	168.963	-2.336	1.00	10.66	A
	ATOM O	1423	O	TYR	A	295	193.387	168.955	-2.741	1.00	11.85	A
60	ATOM N	1424	N	LEU	A	296	195.460	169.797	-2.805	1.00	10.92	A
	ATOM C	1425	CA	LEU	A	296	195.119	170.800	-3.807	1.00	13.78	A

5	ATOM C	1426	CB	LEU A 296	196.328	171.679	-4.144	1.00	11.44	A
	ATOM C	1427	CG	LEU A 296	196.931	172.488	-2.995	1.00	15.78	A
	ATOM C	1428	CD1	LEU A 296	198.287	173.081	-3.411	1.00	13.74	A
	ATOM C	1429	CD2	LEU A 296	195.954	173.585	-2.582	1.00	15.05	A
10	ATOM C	1430	C	LEU A 296	194.591	170.206	-5.108	1.00	14.17	A
	ATOM O	1431	O	LEU A 296	195.144	169.255	-5.648	1.00	12.20	A
15	ATOM N	1432	N	PRO A 297	193.504	170.783	-5.631	1.00	13.56	A
	ATOM C	1433	CD	PRO A 297	192.676	171.841	-5.015	1.00	13.83	A
20	ATOM C	1434	CA	PRO A 297	192.921	170.302	-6.893	1.00	12.38	A
	ATOM C	1435	CB	PRO A 297	191.516	170.923	-6.872	1.00	14.10	A
	ATOM C	1436	CG	PRO A 297	191.744	172.233	-6.155	1.00	13.16	A
	ATOM C	1437	C	PRO A 297	193.772	170.826	-8.083	1.00	14.86	A
25	ATOM O	1438	O	PRO A 297	194.361	171.906	-7.993	1.00	14.20	A
	ATOM N	1439	N	PRO A 298	193.830	170.080	-9.213	1.00	14.90	A
30	ATOM C	1440	CD	PRO A 298	193.074	168.838	-9.478	1.00	13.08	A
	ATOM C	1441	CA	PRO A 298	194.606	170.479	-10.403	1.00	12.06	A
35	ATOM C	1442	CB	PRO A 298	194.228	169.428	-11.450	1.00	12.23	A
	ATOM C	1443	CG	PRO A 298	193.813	168.254	-10.653	1.00	11.96	A
	ATOM C	1444	C	PRO A 298	194.250	171.874	-10.894	1.00	12.75	A
	ATOM O	1445	O	PRO A 298	195.124	172.677	-11.218	1.00	12.47	A
40	ATOM N	1446	N	GLU A 299	192.954	172.154	-10.954	1.00	12.43	A
	ATOM C	1447	CA	GLU A 299	192.495	173.447	-11.427	1.00	15.93	A
45	ATOM C	1448	CB	GLU A 299	190.956	173.520	-11.439	1.00	15.99	A
	ATOM C	1449	CG	GLU A 299	190.283	173.211	-10.098	1.00	20.28	A
50	ATOM C	1450	CD	GLU A 299	189.893	171.729	-9.951	1.00	22.71	A
	ATOM O	1451	OE1	GLU A 299	190.741	170.854	-10.262	1.00	22.72	A
55	ATOM O	1452	OE2	GLU A 299	188.743	171.450	-9.525	1.00	19.63	A
	ATOM C	1453	C	GLU A 299	193.068	174.609	-10.615	1.00	17.99	A
60	ATOM O	1454	O	GLU A 299	193.217	175.706	-11.147	1.00	21.24	A
	ATOM N	1455	N	MET A 300	193.385	174.401	-9.340	1.00	17.80	A
	ATOM C	1456	CA	MET A 300	193.949	175.497	-8.541	1.00	21.17	A

5	ATOM C	1457	CB	MET A 300	193.781	175.248	-7.031	1.00	21.87	A
	ATOM C	1458	CG	MET A 300	192.562	175.935	-6.417	1.00	24.58	A
	ATOM S	1459	SD	MET A 300	192.223	175.516	-4.665	1.00	23.96	A
	ATOM C	1460	CE	MET A 300	193.835	175.427	-4.097	1.00	25.92	A
10	ATOM C	1461	C	MET A 300	195.429	175.697	-8.845	1.00	22.52	A
	ATOM O	1462	O	MET A 300	195.900	176.818	-9.034	1.00	17.97	A
15	ATOM N	1463	N	ILE A 301	196.153	174.592	-8.905	1.00	25.70	A
	ATOM C	1464	CA	ILE A 301	197.573	174.627	-9.160	1.00	28.05	A
20	ATOM C	1465	CB	ILE A 301	198.162	173.192	-9.173	1.00	31.23	A
	ATOM C	1466	CG2	ILE A 301	199.640	173.228	-9.502	1.00	33.00	A
	ATOM C	1467	CG1	ILE A 301	197.977	172.525	-7.813	1.00	34.03	A
	ATOM C	1468	CD1	ILE A 301	198.227	171.019	-7.871	1.00	39.59	A
25	ATOM C	1469	C	ILE A 301	197.857	175.289	-10.501	1.00	28.39	A
	ATOM O	1470	O	ILE A 301	198.736	176.140	-10.608	1.00	28.70	A
30	ATOM N	1471	N	GLU A 302	197.091	174.902	-11.513	1.00	29.15	A
	ATOM C	1472	CA	GLU A 302	197.260	175.411	-12.864	1.00	27.63	A
35	ATOM C	1473	CB	GLU A 302	196.614	174.449	-13.847	1.00	28.51	A
	ATOM C	1474	CG	GLU A 302	197.309	173.128	-13.932	1.00	31.90	A
	ATOM C	1475	CD	GLU A 302	196.442	172.074	-14.604	1.00	34.88	A
40	ATOM O	1476	OE1	GLU A 302	195.546	172.441	-15.420	1.00	35.44	A
	ATOM O	1477	OE2	GLU A 302	196.663	170.878	-14.322	1.00	33.88	A
45	ATOM C	1478	C	GLU A 302	196.759	176.817	-13.160	1.00	26.56	A
	ATOM O	1479	O	GLU A 302	196.730	177.216	-14.323	1.00	25.45	A
50	ATOM N	1480	N	GLY A 303	196.351	177.553	-12.130	1.00	26.68	A
	ATOM C	1481	CA	GLY A 303	195.891	178.915	-12.333	1.00	24.63	A
	ATOM C	1482	C	GLY A 303	194.576	179.072	-13.077	1.00	26.17	A
	ATOM O	1483	O	GLY A 303	194.333	180.080	-13.739	1.00	25.60	A
55	ATOM N	1484	N	ARG A 304	193.718	178.068	-12.976	1.00	27.24	A
	ATOM C	1485	CA	ARG A 304	192.409	178.095	-13.617	1.00	26.83	A
60	ATOM C	1486	CB	ARG A 304	192.068	176.721	-14.229	1.00	26.35	A
	ATOM C	1487	CG	ARG A 304	192.726	176.410	-15.584	1.00	35.40	A

5	ATOM C	1488	CD	ARG	A	304	191.737	176.691	-16.749	1.00	43.36	A
	ATOM N	1489	NE	ARG	A	304	192.316	176.665	-18.095	1.00	47.14	A
	ATOM C	1490	CZ	ARG	A	304	191.602	176.827	-19.210	1.00	51.59	A
	ATOM N	1491	NH1	ARG	A	304	190.290	177.025	-19.121	1.00	54.10	A
10	ATOM N	1492	NH2	ARG	A	304	192.189	176.794	-20.413	1.00	53.71	A
	ATOM C	1493	C	ARG	A	304	191.386	178.429	-12.536	1.00	27.81	A
15	ATOM O	1494	O	ARG	A	304	191.684	178.391	-11.326	1.00	29.71	A
	ATOM N	1495	N	MET	A	305	190.178	178.746	-12.969	1.00	25.68	A
	ATOM C	1496	CA	MET	A	305	189.112	179.048	-12.038	1.00	26.17	A
20	ATOM C	1497	CB	MET	A	305	188.027	179.807	-12.757	1.00	30.29	A
	ATOM C	1498	CG	MET	A	305	188.517	181.155	-13.154	1.00	35.60	A
25	ATOM S	1499	SD	MET	A	305	187.192	182.156	-13.740	1.00	46.48	A
	ATOM C	1500	CE	MET	A	305	187.949	182.896	-15.291	1.00	45.95	A
	ATOM C	1501	C	MET	A	305	188.544	177.772	-11.466	1.00	23.39	A
30	ATOM O	1502	O	MET	A	305	188.653	176.721	-12.082	1.00	23.54	A
	ATOM N	1503	N	HIS	A	306	187.934	177.852	-10.290	1.00	21.16	A
35	ATOM C	1504	CA	HIS	A	306	187.363	176.655	-9.703	1.00	17.32	A
	ATOM C	1505	CB	HIS	A	306	188.312	176.035	-8.671	1.00	15.79	A
	ATOM C	1506	CG	HIS	A	306	188.498	176.853	-7.431	1.00	14.36	A
40	ATOM C	1507	CD2	HIS	A	306	187.895	176.788	-6.218	1.00	12.29	A
	ATOM N	1508	ND1	HIS	A	306	189.411	177.880	-7.347	1.00	15.91	A
45	ATOM C	1509	CE1	HIS	A	306	189.366	178.411	-6.139	1.00	13.45	A
	ATOM N	1510	NE2	HIS	A	306	188.453	177.767	-5.434	1.00	10.38	A
	ATOM C	1511	C	HIS	A	306	186.000	176.913	-9.078	1.00	18.65	A
50	ATOM O	1512	O	HIS	A	306	185.528	178.063	-9.040	1.00	15.46	A
	ATOM N	1513	N	ASP	A	307	185.376	175.822	-8.622	1.00	18.40	A
55	ATOM C	1514	CA	ASP	A	307	184.057	175.824	-7.986	1.00	20.30	A
	ATOM C	1515	CB	ASP	A	307	182.969	175.631	-9.035	1.00	24.34	A
	ATOM C	1516	CG	ASP	A	307	183.174	174.374	-9.865	1.00	30.83	A
60	ATOM O	1517	OD1	ASP	A	307	183.553	173.321	-9.286	1.00	33.25	A
	ATOM O	1518	OD2	ASP	A	307	182.949	174.430	-11.098	1.00	33.88	A

5	ATOM C	1519	C	ASP A	307	183.948	174.721	-6.917	1.00	19.00	A
	ATOM O	1520	O	ASP A	307	184.973	174.176	-6.486	1.00	21.60	A
10	ATOM N	1521	N	GLU A	308	182.720	174.368	-6.519	1.00	18.46	A
	ATOM C	1522	CA	GLU A	308	182.507	173.358	-5.479	1.00	17.19	A
15	ATOM C	1523	CB	GLU A	308	181.014	173.257	-5.075	1.00	19.78	A
	ATOM C	1524	CG	GLU A	308	180.067	172.849	-6.190	1.00	29.00	A
20	ATOM C	1525	CD	GLU A	308	178.600	172.827	-5.777	1.00	33.58	A
	ATOM O	1526	OE1	GLU A	308	178.121	173.800	-5.139	1.00	38.06	A
25	ATOM O	1527	OE2	GLU A	308	177.910	171.836	-6.115	1.00	41.55	A
	ATOM C	1528	C	GLU A	308	183.048	171.977	-5.820	1.00	14.99	A
30	ATOM O	1529	O	GLU A	308	183.135	171.106	-4.946	1.00	14.14	A
	ATOM N	1530	N	LYS A	309	183.452	171.780	-7.066	1.00	12.83	A
35	ATOM C	1531	CA	LYS A	309	183.997	170.488	-7.449	1.00	16.26	A
	ATOM C	1532	CB	LYS A	309	184.061	170.376	-8.972	1.00	18.82	A
40	ATOM C	1533	CG	LYS A	309	182.731	170.086	-9.593	1.00	21.29	A
	ATOM C	1534	CD	LYS A	309	182.215	168.769	-9.041	1.00	29.52	A
45	ATOM C	1535	CE	LYS A	309	181.020	168.263	-9.842	1.00	30.17	A
	ATOM N	1536	NZ	LYS A	309	180.649	166.912	-9.358	1.00	35.57	A
50	ATOM C	1537	C	LYS A	309	185.370	170.202	-6.826	1.00	16.49	A
	ATOM O	1538	O	LYS A	309	185.816	169.051	-6.804	1.00	15.73	A
55	ATOM N	1539	N	VAL A	310	186.025	171.233	-6.291	1.00	15.44	A
	ATOM C	1540	CA	VAL A	310	187.319	171.020	-5.662	1.00	13.90	A
60	ATOM C	1541	CB	VAL A	310	188.051	172.358	-5.281	1.00	15.52	A
	ATOM C	1542	CG1	VAL A	310	188.197	173.247	-6.503	1.00	7.36	A
65	ATOM C	1543	CG2	VAL A	310	187.332	173.065	-4.151	1.00	12.70	A
	ATOM C	1544	C	VAL A	310	187.132	170.159	-4.410	1.00	17.23	A
70	ATOM O	1545	O	VAL A	310	188.008	169.357	-4.083	1.00	19.39	A
	ATOM N	1546	N	ASP A	311	186.013	170.306	-3.700	1.00	14.90	A
75	ATOM C	1547	CA	ASP A	311	185.804	169.452	-2.541	1.00	14.20	A
	ATOM C	1548	CB	ASP A	311	184.574	169.876	-1.727	1.00	16.81	A
80	ATOM C	1549	CG	ASP A	311	184.778	171.192	-0.974	1.00	16.28	A

5	ATOM O	1550	OD1	ASP	A	311	185.950	171.565	-0.731	1.00	12.12	A
	ATOM O	1551	OD2	ASP	A	311	183.756	171.832	-0.617	1.00	13.33	A
	ATOM C	1552	C	ASP	A	311	185.640	167.983	-2.979	1.00	14.98	A
	ATOM O	1553	O	ASP	A	311	185.953	167.090	-2.202	1.00	16.71	A
10	ATOM N	1554	N	LEU	A	312	185.162	167.723	-4.205	1.00	13.32	A
	ATOM C	1555	CA	LEU	A	312	185.019	166.342	-4.703	1.00	13.83	A
15	ATOM C	1556	CB	LEU	A	312	184.238	166.279	-6.028	1.00	12.75	A
	ATOM C	1557	CG	LEU	A	312	182.708	166.216	-6.008	1.00	16.02	A
20	ATOM C	1558	CD1	LEU	A	312	182.269	164.959	-5.273	1.00	14.12	A
	ATOM C	1559	CD2	LEU	A	312	182.118	167.482	-5.336	1.00	16.09	A
	ATOM C	1560	C	LEU	A	312	186.399	165.749	-4.951	1.00	13.94	A
	ATOM O	1561	O	LEU	A	312	186.616	164.546	-4.837	1.00	15.77	A
25	ATOM N	1562	N	TRP	A	313	187.338	166.594	-5.329	1.00	15.19	A
	ATOM C	1563	CA	TRP	A	313	188.673	166.093	-5.553	1.00	13.67	A
30	ATOM C	1564	CB	TRP	A	313	189.505	167.131	-6.287	1.00	10.13	A
	ATOM C	1565	CG	TRP	A	313	190.948	166.889	-6.208	1.00	9.91	A
35	ATOM C	1566	CD2	TRP	A	313	191.775	166.296	-7.214	1.00	11.32	A
	ATOM C	1567	CE2	TRP	A	313	193.109	166.370	-6.750	1.00	10.99	A
	ATOM C	1568	CE3	TRP	A	313	191.523	165.729	-8.471	1.00	8.98	A
	ATOM C	1569	CD1	TRP	A	313	191.784	167.266	-5.199	1.00	10.59	A
40	ATOM N	1570	NE1	TRP	A	313	193.083	166.960	-5.513	1.00	9.03	A
	ATOM C	1571	CZ2	TRP	A	313	194.190	165.890	-7.494	1.00	10.17	A
45	ATOM C	1572	CZ3	TRP	A	313	192.598	165.254	-9.214	1.00	13.43	A
	ATOM C	1573	CH2	TRP	A	313	193.923	165.344	-8.723	1.00	12.05	A
50	ATOM C	1574	C	TRP	A	313	189.258	165.776	-4.183	1.00	12.20	A
	ATOM O	1575	O	TRP	A	313	189.803	164.704	-3.983	1.00	11.38	A
55	ATOM N	1576	N	SER	A	314	189.111	166.700	-3.236	1.00	13.68	A
	ATOM C	1577	CA	SER	A	314	189.636	166.492	-1.893	1.00	16.07	A
	ATOM C	1578	CB	SER	A	314	189.229	167.643	-0.984	1.00	17.53	A
60	ATOM O	1579	OG	SER	A	314	190.261	168.612	-0.972	1.00	25.41	A
	ATOM C	1580	C	SER	A	314	189.172	165.168	-1.283	1.00	16.32	A

5	ATOM O	1581	O	SER A 314	189.942	164.475	-0.628	1.00	15.29	A
	ATOM N	1582	N	LEU A 315	187.907	164.838	-1.517	1.00	15.55	A
	ATOM C	1583	CA	LEU A 315	187.311	163.618	-1.029	1.00	15.03	A
	ATOM C	1584	CB	LEU A 315	185.822	163.597	-1.392	1.00	15.51	A
10	ATOM C	1585	CG	LEU A 315	184.951	162.599	-0.624	1.00	17.84	A
	ATOM C	1586	CD1	LEU A 315	184.877	163.015	0.840	1.00	17.24	A
15	ATOM C	1587	CD2	LEU A 315	183.555	162.551	-1.222	1.00	15.53	A
	ATOM C	1588	C	LEU A 315	188.031	162.402	-1.626	1.00	15.76	A
20	ATOM O	1589	O	LEU A 315	188.237	161.399	-0.935	1.00	16.26	A
	ATOM N	1590	N	GLY A 316	188.414	162.480	-2.899	1.00	13.03	A
	ATOM C	1591	CA	GLY A 316	189.109	161.357	-3.507	1.00	12.73	A
	ATOM C	1592	C	GLY A 316	190.486	161.200	-2.878	1.00	13.41	A
25	ATOM O	1593	O	GLY A 316	190.933	160.092	-2.576	1.00	11.78	A
	ATOM N	1594	N	VAL A 317	191.167	162.329	-2.702	1.00	12.49	A
30	ATOM C	1595	CA	VAL A 317	192.481	162.351	-2.089	1.00	11.35	A
	ATOM C	1596	CB	VAL A 317	193.034	163.812	-1.984	1.00	11.65	A
35	ATOM C	1597	CG1	VAL A 317	194.231	163.859	-1.079	1.00	10.54	A
	ATOM C	1598	CG2	VAL A 317	193.431	164.323	-3.360	1.00	8.84	A
	ATOM C	1599	C	VAL A 317	192.362	161.759	-0.680	1.00	12.97	A
40	ATOM O	1600	O	VAL A 317	193.152	160.887	-0.280	1.00	11.80	A
	ATOM N	1601	N	LEU A 318	191.355	162.229	0.052	1.00	10.99	A
45	ATOM C	1602	CA	LEU A 318	191.097	161.785	1.408	1.00	12.40	A
	ATOM C	1603	CB	LEU A 318	189.958	162.618	2.007	1.00	15.26	A
	ATOM C	1604	CG	LEU A 318	189.652	162.340	3.475	1.00	15.97	A
50	ATOM C	1605	CD1	LEU A 318	190.731	162.990	4.377	1.00	14.54	A
	ATOM C	1606	CD2	LEU A 318	188.310	162.873	3.783	1.00	13.89	A
55	ATOM C	1607	C	LEU A 318	190.760	160.286	1.527	1.00	12.64	A
	ATOM O	1608	O	LEU A 318	191.232	159.610	2.437	1.00	10.92	A
	ATOM N	1609	N	CYS A 319	189.936	159.778	0.617	1.00	12.91	A
60	ATOM C	1610	CA	CYS A 319	189.547	158.372	0.623	1.00	15.63	A
	ATOM C	1611	CB	CYS A 319	188.512	158.092	-0.479	1.00	20.57	A

5	ATOM S	1612	SG	CYS A 319	187.933	156.363	-0.531	1.00	23.04	A
	ATOM C	1613	C	CYS A 319	190.757	157.490	0.394	1.00	15.66	A
10	ATOM O	1614	O	CYS A 319	190.906	156.439	1.025	1.00	15.68	A
	ATOM N	1615	N	TYR A 320	191.614	157.922	-0.527	1.00	13.11	A
15	ATOM C	1616	CA	TYR A 320	192.833	157.194	-0.827	1.00	12.42	A
	ATOM C	1617	CB	TYR A 320	193.560	157.870	-1.999	1.00	12.90	A
20	ATOM C	1618	CG	TYR A 320	194.879	157.235	-2.378	1.00	11.79	A
	ATOM C	1619	CD1	TYR A 320	196.014	157.423	-1.594	1.00	11.63	A
25	ATOM C	1620	CE1	TYR A 320	197.213	156.803	-1.906	1.00	13.39	A
	ATOM C	1621	CD2	TYR A 320	194.978	156.414	-3.495	1.00	13.02	A
30	ATOM C	1622	CE2	TYR A 320	196.167	155.790	-3.822	1.00	14.81	A
	ATOM C	1623	CZ	TYR A 320	197.287	155.980	-3.023	1.00	16.61	A
35	ATOM O	1624	OH	TYR A 320	198.459	155.299	-3.325	1.00	14.17	A
	ATOM C	1625	C	TYR A 320	193.727	157.138	0.428	1.00	13.58	A
40	ATOM O	1626	O	TYR A 320	194.217	156.062	0.797	1.00	12.75	A
	ATOM N	1627	N	GLU A 321	193.922	158.287	1.083	1.00	12.98	A
45	ATOM C	1628	CA	GLU A 321	194.752	158.359	2.289	1.00	13.87	A
	ATOM C	1629	CB	GLU A 321	194.858	159.798	2.815	1.00	15.03	A
50	ATOM C	1630	CG	GLU A 321	196.109	160.011	3.685	1.00	22.02	A
	ATOM C	1631	CD	GLU A 321	196.204	161.394	4.326	1.00	27.52	A
55	ATOM O	1632	OE1	GLU A 321	195.889	162.413	3.676	1.00	30.94	A
	ATOM O	1633	OE2	GLU A 321	196.621	161.470	5.494	1.00	31.35	A
60	ATOM C	1634	C	GLU A 321	194.218	157.470	3.416	1.00	14.01	A
	ATOM O	1635	O	GLU A 321	194.986	156.877	4.166	1.00	14.13	A
65	ATOM N	1636	N	PHE A 322	192.899	157.384	3.536	1.00	13.55	A
	ATOM C	1637	CA	PHE A 322	192.291	156.568	4.576	1.00	12.09	A
70	ATOM C	1638	CB	PHE A 322	190.765	156.710	4.570	1.00	6.70	A
	ATOM C	1639	CG	PHE A 322	190.272	157.975	5.176	1.00	6.79	A
75	ATOM C	1640	CD1	PHE A 322	191.144	158.836	5.838	1.00	7.89	A
	ATOM C	1641	CD2	PHE A 322	188.933	158.312	5.106	1.00	8.09	A
80	ATOM C	1642	CE1	PHE A 322	190.688	160.011	6.416	1.00	6.90	A

5	ATOM C	1643	CE2	PHE A 322	188.464	159.497	5.689	1.00	10.00	A
	ATOM C	1644	CZ	PHE A 322	189.346	160.340	6.345	1.00	8.24	A
	ATOM C	1645	C	PHE A 322	192.629	155.107	4.398	1.00	12.56	A
	ATOM O	1646	O	PHE A 322	192.888	154.401	5.375	1.00	14.57	A
10	ATOM N	1647	N	LEU A 323	192.629	154.663	3.147	1.00	11.23	A
	ATOM C	1648	CA	LEU A 323	192.876	153.269	2.830	1.00	10.81	A
15	ATOM C	1649	CB	LEU A 323	192.181	152.923	1.510	1.00	11.58	A
	ATOM C	1650	CG	LEU A 323	190.650	152.911	1.467	1.00	11.82	A
20	ATOM C	1651	CD1	LEU A 323	190.149	152.693	0.033	1.00	1.00	A
	ATOM C	1652	CD2	LEU A 323	190.158	151.799	2.429	1.00	8.83	A
	ATOM C	1653	C	LEU A 323	194.3	152.888	2.725	1.00	13.31	A
	ATOM O	1654	O	LEU A 323	194.734	151.769	3.072	1.00	13.08	A
25	ATOM N	1655	N	VAL A 324	195.144	153.832	2.253	1.00	13.79	A
	ATOM C	1656	CA	VAL A 324	196.552	153.589	2.028	1.00	13.43	A
30	ATOM C	1657	CB	VAL A 324	196.958	154.241	0.703	1.00	13.53	A
	ATOM C	1658	CG1	VAL A 324	198.387	153.909	0.365	1.00	10.33	A
35	ATOM C	1659	CG2	VAL A 324	196.009	153.788	-0.384	1.00	10.31	A
	ATOM C	1660	C	VAL A 324	197.439	154.085	3.153	1.00	15.36	A
	ATOM O	1661	O	VAL A 324	198.496	153.525	3.419	1.00	15.10	A
40	ATOM N	1662	N	GLY A 325	197.019	155.146	3.819	1.00	16.58	A
	ATOM C	1663	CA	GLY A 325	197.834	155.647	4.902	1.00	18.98	A
45	ATOM C	1664	C	GLY A 325	198.687	156.819	4.459	1.00	22.31	A
	ATOM O	1665	O	GLY A 325	199.484	157.330	5.245	1.00	22.91	A
50	ATOM N	1666	N	LYS A 326	198.556	157.238	3.204	1.00	22.34	A
	ATOM C	1667	CA	LYS A 326	199.299	158.399	2.743	1.00	20.73	A
	ATOM C	1668	CB	LYS A 326	200.775	158.057	2.468	1.00	22.54	A
	ATOM C	1669	CG	LYS A 326	201.002	157.016	1.405	1.00	26.76	A
55	ATOM C	1670	CD	LYS A 326	202.478	156.728	1.181	1.00	29.37	A
	ATOM C	1671	CE	LYS A 326	202.635	155.634	0.108	1.00	36.99	A
60	ATOM N	1672	NZ	LYS A 326	204.059	155.235	-0.146	1.00	40.73	A
	ATOM C	1673	C	LYS A 326	198.627	158.927	1.496	1.00	18.10	A

[illegible]

5	ATOM O	1705	OE1	GLU	A	330	203.825	161.798	2.890	1.00	43.93	A
	ATOM O	1706	OE2	GLU	A	330	203.186	160.230	1.490	1.00	43.19	A
	ATOM C	1707	C	GLU	A	330	204.404	162.666	-2.593	1.00	25.36	A
	ATOM O	1708	O	GLU	A	330	204.712	161.627	-3.177	1.00	25.32	A
10	ATOM N	1709	N	ALA	A	331	205.195	163.733	-2.551	1.00	23.31	A
	ATOM C	1710	CA	ALA	A	331	206.506	163.745	-3.184	1.00	23.23	A
15	ATOM C	1711	CB	ALA	A	331	206.432	164.479	-4.500	1.00	19.73	A
	ATOM C	1712	C	ALA	A	331	207.503	164.429	-2.239	1.00	24.76	A
	ATOM O	1713	O	ALA	A	331	207.109	165.040	-1.249	1.00	22.52	A
20	ATOM N	1714	N	ASN	A	332	208.794	164.320	-2.542	1.00	27.89	A
	ATOM C	1715	CA	ASN	A	332	209.822	164.922	-1.692	1.00	30.47	A
25	ATOM C	1716	CB	ASN	A	332	211.174	164.246	-1.975	1.00	32.87	A
	ATOM C	1717	CG	ASN	A	332	211.190	162.794	-1.504	1.00	37.45	A
30	ATOM O	1718	OD1	ASN	A	332	210.716	162.504	-0.401	1.00	36.73	A
	ATOM N	1719	ND2	ASN	A	332	211.729	161.883	-2.321	1.00	37.38	A
	ATOM C	1720	C	ASN	A	332	209.942	166.462	-1.771	1.00	29.91	A
35	ATOM O	1721	O	ASN	A	332	210.601	167.073	-0.928	1.00	29.72	A
	ATOM N	1722	N	THR	A	333	209.303	167.092	-2.754	1.00	27.34	A
40	ATOM C	1723	CA	THR	A	333	209.369	168.544	-2.881	1.00	25.63	A
	ATOM C	1724	CB	THR	A	333	210.411	168.968	-3.919	1.00	27.29	A
	ATOM O	1725	OG1	THR	A	333	209.862	168.766	-5.232	1.00	25.31	A
45	ATOM C	1726	CG2	THR	A	333	211.683	168.122	-3.769	1.00	28.40	A
	ATOM C	1727	C	THR	A	333	208.021	169.099	-3.341	1.00	24.25	A
50	ATOM O	1728	O	THR	A	333	207.168	168.355	-3.832	1.00	24.65	A
	ATOM N	1729	N	TYR	A	334	207.839	170.406	-3.177	1.00	22.97	A
	ATOM C	1730	CA	TYR	A	334	206.610	171.081	-3.584	1.00	24.27	A
55	ATOM C	1731	CB	TYR	A	334	206.670	172.557	-3.243	1.00	26.40	A
	ATOM C	1732	CG	TYR	A	334	206.122	172.899	-1.885	1.00	28.73	A
60	ATOM C	1733	CD1	TYR	A	334	206.846	172.639	-0.725	1.00	29.53	A
	ATOM C	1734	CE1	TYR	A	334	206.322	172.945	0.537	1.00	32.11	A
	ATOM C	1735	CD2	TYR	A	334	204.863	173.476	-1.759	1.00	28.50	A

5	ATOM C	1736	CE2	TYR A 334	204.329	173.794	-0.497	1.00	29.43	A
	ATOM C	1737	CZ	TYR A 334	205.072	173.518	0.645	1.00	31.88	A
	ATOM O	1738	OH	TYR A 334	204.597	173.783	1.910	1.00	34.80	A
	ATOM C	1739	C	TYR A 334	206.379	170.979	-5.088	1.00	25.01	A
10	ATOM O	1740	O	TYR A 334	205.267	170.712	-5.567	1.00	24.09	A
	ATOM N	1741	N	GLN A 335	207.445	171.221	-5.831	1.00	24.15	A
15	ATOM C	1742	CA	GLN A 335	207.401	171.183	-7.272	1.00	26.26	A
	ATOM C	1743	CB	GLN A 335	208.763	171.616	-7.820	1.00	30.16	A
	ATOM C	1744	CG	GLN A 335	208.690	172.407	-9.123	1.00	37.20	A
20	ATOM C	1745	CD	GLN A 335	209.938	173.249	-9.353	1.00	44.29	A
	ATOM O	1746	OE1	GLN A 335	211.075	172.716	-9.361	1.00	45.86	A
25	ATOM N	1747	NE2	GLN A 335	209.749	174.581	-9.540	1.00	45.65	A
	ATOM C	1748	C	GLN A 335	207.014	169.785	-7.766	1.00	24.06	A
	ATOM O	1749	O	GLN A 335	206.182	169.643	-8.661	1.00	20.60	A
30	ATOM N	1750	N	GLU A 336	207.596	168.746	-7.179	1.00	23.21	A
	ATOM C	1751	CA	GLU A 336	207.243	167.407	-7.624	1.00	22.61	A
35	ATOM C	1752	CB	GLU A 336	208.183	166.360	-7.022	1.00	19.74	A
	ATOM C	1753	CG	GLU A 336	207.807	164.932	-7.350	1.00	27.97	A
	ATOM C	1754	CD	GLU A 336	207.852	164.603	-8.845	1.00	35.28	A
40	ATOM O	1755	OE1	GLU A 336	207.231	163.579	-9.236	1.00	38.15	A
	ATOM O	1756	OE2	GLU A 336	208.508	165.350	-9.628	1.00	39.74	A
45	ATOM C	1757	C	GLU A 336	205.775	167.056	-7.327	1.00	23.14	A
	ATOM O	1758	O	GLU A 336	205.138	166.363	-8.124	1.00	23.03	A
	ATOM N	1759	N	THR A 337	205.241	167.517	-6.196	1.00	21.09	A
50	ATOM C	1760	CA	THR A 337	203.849	167.229	-5.868	1.00	21.21	A
	ATOM C	1761	CB	THR A 337	203.541	167.589	-4.380	1.00	22.66	A
55	ATOM O	1762	OG1	THR A 337	204.334	166.744	-3.537	1.00	24.71	A
	ATOM C	1763	CG2	THR A 337	202.072	167.366	-4.030	1.00	16.15	A
	ATOM C	1764	C	THR A 337	202.918	167.944	-6.855	1.00	19.71	A
60	ATOM O	1765	O	THR A 337	201.978	167.329	-7.346	1.00	21.88	A
	ATOM N	1766	N	TYR A 338	203.191	169.210	-7.171	1.00	17.76	A

5	ATOM C	1767	CA	TYR	A	338	202.404	169.982	-8.151	1.00	17.94	A
	ATOM C	1768	CB	TYR	A	338	203.051	171.348	-8.416	1.00	19.72	A
	ATOM C	1769	CG	TYR	A	338	202.924	172.309	-7.282	1.00	21.47	A
	ATOM C	1770	CD1	TYR	A	338	203.927	173.231	-7.014	1.00	26.12	A
	ATOM C	1771	CE1	TYR	A	338	203.780	174.172	-6.003	1.00	31.99	A
10	ATOM C	1772	CD2	TYR	A	338	201.775	172.333	-6.506	1.00	23.72	A
	ATOM C	1773	CE2	TYR	A	338	201.609	173.256	-5.498	1.00	28.25	A
15	ATOM C	1774	CZ	TYR	A	338	202.605	174.184	-5.255	1.00	32.26	A
	ATOM O	1775	OH	TYR	A	338	202.398	175.197	-4.343	1.00	37.49	A
20	ATOM C	1776	C	TYR	A	338	202.342	169.248	-9.480	1.00	17.24	A
	ATOM O	1777	O	TYR	A	338	201.303	169.202	-10.143	1.00	17.93	A
25	ATOM N	1778	N	LYS	A	339	203.492	168.704	-9.869	1.00	18.06	A
	ATOM C	1779	CA	LYS	A	339	203.635	167.967	-11.112	1.00	15.13	A
	ATOM C	1780	CB	LYS	A	339	205.087	167.521	-11.318	1.00	15.66	A
30	ATOM C	1781	CG	LYS	A	339	205.282	166.761	-12.647	1.00	25.11	A
	ATOM C	1782	CD	LYS	A	339	206.675	166.164	-12.838	1.00	28.61	A
	ATOM C	1783	CE	LYS	A	339	207.736	167.232	-12.973	1.00	30.48	A
35	ATOM N	1784	NZ	LYS	A	339	209.081	166.590	-13.128	1.00	37.06	A
	ATOM C	1785	C	LYS	A	339	202.734	166.747	-11.110	1.00	15.66	A
40	ATOM O	1786	O	LYS	A	339	201.999	166.520	-12.062	1.00	16.79	A
	ATOM N	1787	N	ARG	A	340	202.788	165.963	-10.038	1.00	14.01	A
45	ATOM C	1788	CA	ARG	A	340	201.980	164.754	-9.941	1.00	17.25	A
	ATOM C	1789	CB	ARG	A	340	202.444	163.917	-8.749	1.00	17.92	A
	ATOM C	1790	CG	ARG	A	340	203.675	163.112	-9.058	1.00	20.94	A
50	ATOM C	1791	CD	ARG	A	340	204.273	162.632	-7.805	1.00	26.11	A
	ATOM N	1792	NE	ARG	A	340	205.579	162.024	-8.000	1.00	30.74	A
55	ATOM C	1793	CZ	ARG	A	340	206.247	161.430	-7.014	1.00	34.14	A
	ATOM N	1794	NH1	ARG	A	340	205.697	161.387	-5.805	1.00	36.45	A
60	ATOM N	1795	NH2	ARG	A	340	207.447	160.886	-7.219	1.00	32.82	A
	ATOM C	1796	C	ARG	A	340	200.467	164.980	-9.876	1.00	16.32	A
	ATOM O	1797	O	ARG	A	340	199.692	164.177	-10.393	1.00	13.54	A

5	ATOM N	1798	N	ILE A 341	200.052	166.068	-9.242	1.00	16.44	A
	ATOM C	1799	CA	ILE A 341	198.637	166.396	-9.147	1.00	15.90	A
	ATOM C	1800	CB	ILE A 341	198.425	167.544	-8.133	1.00	14.61	A
	ATOM C	1801	CG2	ILE A 341	197.031	168.173	-8.284	1.00	10.21	A
10	ATOM C	1802	CG1	ILE A 341	198.636	166.991	-6.722	1.00	9.86	A
	ATOM C	1803	CD1	ILE A 341	198.865	168.066	-5.710	1.00	10.30	A
15	ATOM C	1804	C	ILE A 341	198.139	166.813	-10.524	1.00	16.94	A
	ATOM O	1805	O	ILE A 341	197.099	166.346	-11.003	1.00	15.49	A
20	ATOM N	1806	N	SER A 342	198.911	167.677	-11.165	1.00	17.49	A
	ATOM C	1807	CA	SER A 342	198.556	168.185	-12.479	1.00	19.50	A
	ATOM C	1808	CB	SER A 342	199.638	169.153	-12.927	1.00	19.12	A
	ATOM O	1809	OG	SER A 342	199.178	169.899	-14.023	1.00	28.84	A
25	ATOM C	1810	C	SER A 342	198.385	167.065	-13.518	1.00	18.65	A
	ATOM O	1811	O	SER A 342	197.544	167.157	-14.414	1.00	17.15	A
30	ATOM N	1812	N	ARG A 343	199.209	166.027	-13.391	1.00	16.76	A
	ATOM C	1813	CA	ARG A 343	199.187	164.881	-14.291	1.00	16.82	A
35	ATOM C	1814	CB	ARG A 343	200.563	164.214	-14.356	1.00	19.40	A
	ATOM C	1815	CG	ARG A 343	201.744	165.034	-14.873	1.00	20.85	A
	ATOM C	1816	CD	ARG A 343	202.986	164.139	-14.768	1.00	22.63	A
	ATOM N	1817	NE	ARG A 343	204.181	164.667	-15.420	1.00	29.67	A
40	ATOM C	1818	CZ	ARG A 343	205.296	163.964	-15.619	1.00	29.30	A
	ATOM N	1819	NH1	ARG A 343	205.362	162.702	-15.211	1.00	27.60	A
45	ATOM N	1820	NH2	ARG A 343	206.337	164.521	-16.239	1.00	30.90	A
	ATOM C	1821	C	ARG A 343	198.213	163.833	-13.749	1.00	17.95	A
50	ATOM O	1822	O	ARG A 343	197.789	162.927	-14.470	1.00	18.61	A
	ATOM N	1823	N	VAL A 344	197.880	163.963	-12.465	1.00	16.47	A
55	ATOM C	1824	CA	VAL A 344	197.014	163.027	-11.767	1.00	15.15	A
	ATOM C	1825	CB	VAL A 344	195.644	162.882	-12.427	1.00	14.04	A
	ATOM C	1826	CG1	VAL A 344	194.791	161.919	-11.603	1.00	14.73	A
60	ATOM C	1827	CG2	VAL A 344	194.949	164.217	-12.503	1.00	14.41	A
	ATOM C	1828	C	VAL A 344	197.751	161.702	-11.847	1.00	19.48	A

5	ATOM O	1829	O	VAL	A	344	197.240	160.697	-12.362	1.00	17.59	A
	ATOM N	1830	N	GLU	A	345	198.970	161.733	-11.320	1.00	20.63	A
	ATOM C	1831	CA	GLU	A	345	199.883	160.600	-11.314	1.00	21.68	A
	ATOM C	1832	CB	GLU	A	345	201.297	161.116	-11.635	1.00	22.57	A
10	ATOM C	1833	CG	GLU	A	345	202.291	160.066	-12.115	1.00	29.02	A
	ATOM C	1834	CD	GLU	A	345	203.609	160.693	-12.596	1.00	34.43	A
15	ATOM O	1835	OE1	GLU	A	345	203.572	161.826	-13.143	1.00	41.54	A
	ATOM O	1836	OE2	GLU	A	345	204.677	160.062	-12.448	1.00	34.88	A
	ATOM C	1837	C	GLU	A	345	199.906	159.839	-9.990	1.00	21.02	A
20	ATOM O	1838	O	GLU	A	345	200.516	160.289	-9.009	1.00	22.86	A
	ATOM N	1839	N	PHE	A	346	199.260	158.679	-9.953	1.00	20.71	A
25	ATOM C	1840	CA	PHE	A	346	199.268	157.868	-8.730	1.00	20.54	A
	ATOM C	1841	CB	PHE	A	346	198.272	158.454	-7.705	1.00	19.53	A
	ATOM C	1842	CG	PHE	A	346	196.835	158.138	-8.013	1.00	21.11	A
30	ATOM C	1843	CD1	PHE	A	346	196.203	157.064	-7.403	1.00	22.02	A
	ATOM C	1844	CD2	PHE	A	346	196.130	158.888	-8.936	1.00	18.36	A
35	ATOM C	1845	CE1	PHE	A	346	194.878	156.744	-7.713	1.00	24.10	A
	ATOM C	1846	CE2	PHE	A	346	194.807	158.574	-9.253	1.00	23.07	A
	ATOM C	1847	CZ	PHE	A	346	194.181	157.500	-8.640	1.00	22.64	A
40	ATOM C	1848	C	PHE	A	346	198.893	156.424	-9.065	1.00	19.41	A
	ATOM O	1849	O	PHE	A	346	198.376	156.142	-10.153	1.00	21.26	A
45	ATOM N	1850	N	THR	A	347	199.158	155.512	-8.137	1.00	17.51	A
	ATOM C	1851	CA	THR	A	347	198.809	154.113	-8.335	1.00	15.60	A
	ATOM C	1852	CB	THR	A	347	200.042	153.259	-8.736	1.00	17.00	A
50	ATOM O	1853	OG1	THR	A	347	201.113	153.494	-7.812	1.00	20.54	A
	ATOM C	1854	CG2	THR	A	347	200.506	153.617	-10.145	1.00	14.88	A
55	ATOM C	1855	C	THR	A	347	198.245	153.623	-7.026	1.00	14.01	A
	ATOM O	1856	O	THR	A	347	198.322	154.324	-6.030	1.00	14.17	A
	ATOM N	1857	N	PHE	A	348	197.659	152.434	-7.029	1.00	14.30	A
60	ATOM C	1858	CA	PHE	A	348	197.097	151.875	-5.809	1.00	15.62	A
	ATOM C	1859	CB	PHE	A	348	195.673	151.335	-6.022	1.00	13.71	A

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5	ATOM C	1891	CZ	PHE A 351	197.128	149.417	1.515	1.00	20.15	A
	ATOM C	1892	C	PHE A 351	193.883	146.509	-1.382	1.00	24.86	A
	ATOM O	1893	O	PHE A 351	192.826	146.215	-0.820	1.00	26.36	A
	ATOM N	1894	N	VAL A 352	193.999	147.575	-2.174	1.00	22.98	A
10	ATOM C	1895	CA	VAL A 352	192.845	148.431	-2.428	1.00	22.53	A
	ATOM C	1896	CB	VAL A 352	193.297	149.810	-2.976	1.00	19.91	A
15	ATOM C	1897	CG1	VAL A 352	192.105	150.680	-3.293	1.00	15.94	A
	ATOM C	1898	CG2	VAL A 352	194.164	150.489	-1.936	1.00	17.58	A
	ATOM C	1899	C	VAL A 352	191.941	147.702	-3.416	1.00	22.85	A
20	ATOM O	1900	O	VAL A 352	192.351	147.406	-4.541	1.00	25.56	A
	ATOM N	1901	N	THR A 353	190.722	147.393	-2.985	1.00	20.20	A
25	ATOM C	1902	CA	THR A 353	189.786	146.668	-3.833	1.00	20.47	A
	ATOM C	1903	CB	THR A 353	188.530	146.264	-3.059	1.00	18.44	A
	ATOM O	1904	OG1	THR A 353	187.777	147.445	-2.740	1.00	19.14	A
30	ATOM C	1905	CG2	THR A 353	188.915	145.544	-1.786	1.00	15.00	A
	ATOM C	1906	C	THR A 353	189.331	147.452	-5.049	1.00	23.02	A
35	ATOM O	1907	O	THR A 353	189.525	148.665	-5.144	1.00	21.93	A
	ATOM N	1908	N	GLU A 354	188.685	146.733	-5.960	1.00	23.98	A
	ATOM C	1909	CA	GLU A 354	188.175	147.274	-7.208	1.00	25.43	A
40	ATOM C	1910	CB	GLU A 354	187.543	146.130	-8.001	1.00	30.21	A
	ATOM C	1911	CG	GLU A 354	186.780	146.540	-9.261	1.00	37.82	A
45	ATOM C	1912	CD	GLU A 354	186.031	145.351	-9.890	1.00	41.79	A
	ATOM O	1913	OE1	GLU A 354	185.501	145.472	-11.025	1.00	43.51	A
	ATOM O	1914	OE2	GLU A 354	185.974	144.281	-9.224	1.00	44.80	A
50	ATOM C	1915	C	GLU A 354	187.175	148.424	-7.055	1.00	24.34	A
	ATOM O	1916	O	GLU A 354	187.182	149.386	-7.840	1.00	24.85	A
55	ATOM N	1917	N	GLY A 355	186.298	148.303	-6.065	1.00	20.96	A
	ATOM C	1918	CA	GLY A 355	185.289	149.314	-5.842	1.00	13.82	A
	ATOM C	1919	C	GLY A 355	185.908	150.595	-5.333	1.00	16.94	A
60	ATOM O	1920	O	GLY A 355	185.529	151.694	-5.760	1.00	13.60	A
	ATOM N	1921	N	ALA A 356	186.868	150.473	-4.425	1.00	15.45	A

5	ATOM C	1922	CA	ALA	A	356	187.501	151.674	-3.909	1.00	19.10	A
	ATOM C	1923	CB	ALA	A	356	188.475	151.326	-2.761	1.00	18.64	A
	ATOM C	1924	C	ALA	A	356	188.235	152.381	-5.068	1.00	19.08	A
	ATOM O	1925	O	ALA	A	356	188.203	153.604	-5.162	1.00	16.84	A
10	ATOM N	1926	N	ARG	A	357	188.874	151.611	-5.951	1.00	18.44	A
	ATOM C	1927	CA	ARG	A	357	189.586	152.184	-7.100	1.00	18.13	A
15	ATOM C	1928	CB	ARG	A	357	190.349	151.113	-7.881	1.00	16.00	A
	ATOM C	1929	CG	ARG	A	357	191.447	150.447	-7.112	1.00	15.75	A
	ATOM C	1930	CD	ARG	A	357	192.125	149.414	-7.941	1.00	14.24	A
20	ATOM N	1931	NE	ARG	A	357	193.120	148.721	-7.139	1.00	18.00	A
	ATOM C	1932	CZ	ARG	A	357	194.249	148.203	-7.607	1.00	18.74	A
25	ATOM N	1933	NH1	ARG	A	357	194.553	148.285	-8.898	1.00	21.62	A
	ATOM N	1934	NH2	ARG	A	357	195.097	147.622	-6.768	1.00	20.49	A
	ATOM C	1935	C	ARG	A	357	188.627	152.856	-8.062	1.00	17.28	A
30	ATOM O	1936	O	ARG	A	357	188.949	153.878	-8.637	1.00	16.53	A
	ATOM N	1937	N	ASP	A	358	187.454	152.272	-8.261	1.00	17.73	A
35	ATOM C	1938	CA	ASP	A	358	186.511	152.887	-9.176	1.00	17.93	A
	ATOM C	1939	CB	ASP	A	358	185.267	152.024	-9.389	1.00	21.16	A
	ATOM C	1940	CG	ASP	A	358	184.269	152.688	-10.327	1.00	23.93	A
40	ATOM O	1941	OD1	ASP	A	358	184.508	152.671	-11.559	1.00	29.93	A
	ATOM O	1942	OD2	ASP	A	358	183.266	153.257	-9.840	1.00	22.82	A
45	ATOM C	1943	C	ASP	A	358	186.081	154.234	-8.611	1.00	17.83	A
	ATOM O	1944	O	ASP	A	358	185.996	155.206	-9.348	1.00	20.18	A
	ATOM N	1945	N	LEU	A	359	185.823	154.299	-7.303	1.00	16.69	A
50	ATOM C	1946	CA	LEU	A	359	185.389	155.543	-6.680	1.00	15.23	A
	ATOM C	1947	CB	LEU	A	359	184.873	155.292	-5.250	1.00	13.90	A
55	ATOM C	1948	CG	LEU	A	359	184.459	156.568	-4.482	1.00	15.76	A
	ATOM C	1949	CD1	LEU	A	359	183.222	157.164	-5.105	1.00	14.16	A
	ATOM C	1950	CD2	LEU	A	359	184.210	156.266	-3.027	1.00	16.19	A
60	ATOM C	1951	C	LEU	A	359	186.478	156.623	-6.646	1.00	15.38	A
	ATOM O	1952	O	LEU	A	359	186.234	157.740	-7.071	1.00	16.61	A

5	ATOM N	1953	N	ILE A 360	187.661	156.300	-6.132	1.00	15.08	A
	ATOM C	1954	CA	ILE A 360	188.737	157.280	-6.054	1.00	16.09	A
	ATOM C	1955	CB	ILE A 360	189.972	156.694	-5.305	1.00	13.18	A
	ATOM C	1956	CG2	ILE A 360	191.132	157.645	-5.348	1.00	8.95	A
	ATOM C	1957	CG1	ILE A 360	189.613	156.445	-3.843	1.00	11.43	A
10	ATOM C	1958	CD1	ILE A 360	190.486	155.406	-3.211	1.00	15.13	A
	ATOM C	1959	C	ILE A 360	189.126	157.752	-7.457	1.00	18.67	A
15	ATOM O	1960	O	ILE A 360	189.433	158.935	-7.652	1.00	19.76	A
	ATOM N	1961	N	SER A 361	189.099	156.841	-8.427	1.00	17.86	A
20	ATOM C	1962	CA	SER A 361	189.437	157.193	-9.792	1.00	17.51	A
	ATOM C	1963	CB	SER A 361	189.511	155.952	-10.682	1.00	18.17	A
25	ATOM O	1964	OG	SER A 361	190.686	155.223	-10.384	1.00	20.30	A
	ATOM C	1965	C	SER A 361	188.438	158.163	-10.382	1.00	18.63	A
30	ATOM O	1966	O	SER A 361	188.805	159.011	-11.209	1.00	19.26	A
	ATOM N	1967	N	ARG A 362	187.175	158.051	-9.977	1.00	18.68	A
35	ATOM C	1968	CA	ARG A 362	186.156	158.973	-10.492	1.00	17.96	A
	ATOM C	1969	CB	ARG A 362	184.740	158.464	-10.227	1.00	18.15	A
40	ATOM C	1970	CG	ARG A 362	184.389	157.189	-10.948	1.00	21.87	A
	ATOM C	1971	CD	ARG A 362	182.950	156.762	-10.710	1.00	24.92	A
45	ATOM N	1972	NE	ARG A 362	182.669	155.532	-11.449	1.00	31.73	A
	ATOM C	1973	CZ	ARG A 362	182.150	155.461	-12.682	1.00	35.25	A
50	ATOM N	1974	NH1	ARG A 362	181.805	156.557	-13.358	1.00	34.91	A
	ATOM N	1975	NH2	ARG A 362	182.052	154.276	-13.281	1.00	35.12	A
55	ATOM C	1976	C	ARG A 362	186.287	160.332	-9.817	1.00	16.66	A
	ATOM O	1977	O	ARG A 362	186.086	161.367	-10.452	1.00	21.59	A
60	ATOM N	1978	N	LEU A 363	186.602	160.348	-8.527	1.00	15.31	A
	ATOM C	1979	CA	LEU A 363	186.726	161.620	-7.814	1.00	15.39	A
	ATOM C	1980	CB	LEU A 363	186.758	161.376	-6.295	1.00	13.54	A
	ATOM C	1981	CG	LEU A 363	185.452	160.880	-5.638	1.00	14.63	A
	ATOM C	1982	CD1	LEU A 363	185.723	160.358	-4.216	1.00	12.73	A
	ATOM C	1983	CD2	LEU A 363	184.423	162.005	-5.613	1.00	7.80	A

5	ATOM C	1984	C	LEU A 363	187.989	162.357	-8.252	1.00	16.50	A
	ATOM O	1985	O	LEU A 363	188.033	163.593	-8.252	1.00	16.60	A
	ATOM N	1986	N	LEU A 364	189.008	161.597	-8.656	1.00	17.23	A
	ATOM C	1987	CA	LEU A 364	190.285	162.182	-9.051	1.00	20.15	A
10	ATOM C	1988	CB	LEU A 364	191.419	161.335	-8.467	1.00	18.29	A
	ATOM C	1989	CG	LEU A 364	191.504	161.377	-6.926	1.00	20.11	A
15	ATOM C	1990	CD1	LEU A 364	192.737	160.607	-6.509	1.00	16.10	A
	ATOM C	1991	CD2	LEU A 364	191.576	162.820	-6.413	1.00	16.30	A
20	ATOM C	1992	C	LEU A 364	190.474	162.393	-10.557	1.00	19.92	A
	ATOM O	1993	O	LEU A 364	191.511	162.052	-11.143	1.00	20.12	A
	ATOM N	1994	N	LYS A 365	189.450	162.967	-11.169	1.00	19.36	A
	ATOM C	1995	CA	LYS A 365	189.461	163.275	-12.581	1.00	19.00	A
25	ATOM C	1996	CB	LYS A 365	188.039	163.289	-13.117	1.00	22.47	A
	ATOM C	1997	CG	LYS A 365	187.417	161.929	-13.243	1.00	23.42	A
30	ATOM C	1998	CD	LYS A 365	188.039	161.224	-14.400	1.00	23.31	A
	ATOM C	1999	CE	LYS A 365	187.320	159.930	-14.693	1.00	24.89	A
35	ATOM N	2000	NZ	LYS A 365	187.970	159.249	-15.851	1.00	30.35	A
	ATOM C	2001	C	LYS A 365	190.039	164.670	-12.715	1.00	18.75	A
	ATOM O	2002	O	LYS A 365	189.654	165.568	-11.956	1.00	15.64	A
40	ATOM N	2003	N	HIS A 366	190.949	164.850	-13.676	1.00	17.07	A
	ATOM C	2004	CA	HIS A 366	191.568	166.150	-13.920	1.00	17.25	A
45	ATOM C	2005	CB	HIS A 366	192.611	166.038	-15.043	1.00	15.66	A
	ATOM C	2006	CG	HIS A 366	193.302	167.331	-15.352	1.00	18.71	A
50	ATOM C	2007	CD2	HIS A 366	194.437	167.877	-14.849	1.00	17.17	A
	ATOM N	2008	ND1	HIS A 366	192.763	168.283	-16.194	1.00	19.79	A
	ATOM C	2009	CE1	HIS A 366	193.530	169.361	-16.187	1.00	18.47	A
55	ATOM N	2010	NE2	HIS A 366	194.552	169.141	-15.378	1.00	18.20	A
	ATOM C	2011	C	HIS A 366	190.493	167.186	-14.291	1.00	17.88	A
60	ATOM O	2012	O	HIS A 366	190.553	168.334	-13.864	1.00	14.94	A
	ATOM N	2013	N	ASN A 367	189.500	166.769	-15.071	1.00	19.37	A
	ATOM C	2014	CA	ASN A 367	188.436	167.676	-15.490	1.00	22.11	A

5	ATOM C	2015	CB	ASN A	367	187.841	167.205	-16.823	1.00	24.11	A
	ATOM C	2016	CG	ASN A	367	186.929	168.246	-17.452	1.00	29.29	A
	ATOM O	2017	OD1	ASN A	367	185.990	168.718	-16.827	1.00	34.30	A
	ATOM N	2018	ND2	ASN A	367	187.209	168.611	-18.688	1.00	31.42	A
10	ATOM C	2019	C	ASN A	367	187.348	167.721	-14.412	1.00	22.00	A
	ATOM O	2020	O	ASN A	367	186.644	166.739	-14.198	1.00	21.37	A
15	ATOM N	2021	N	PRO A	368	187.174	168.881	-13.751	1.00	22.13	A
	ATOM C	2022	CD	PRO A	368	187.763	170.174	-14.151	1.00	21.11	A
20	ATOM C	2023	CA	PRO A	368	186.181	169.073	-12.682	1.00	21.45	A
	ATOM C	2024	CB	PRO A	368	186.292	170.571	-12.377	1.00	23.08	A
	ATOM C	2025	CG	PRO A	368	187.705	170.942	-12.864	1.00	19.70	A
25	ATOM C	2026	C	PRO A	368	184.755	168.638	-13.047	1.00	22.70	A
	ATOM O	2027	O	PRO A	368	184.016	168.091	-12.209	1.00	21.09	A
30	ATOM N	2028	N	SER A	369	184.386	168.865	-14.303	1.00	21.10	A
	ATOM C	2029	CA	SER A	369	183.068	168.492	-14.818	1.00	25.15	A
	ATOM C	2030	CB	SER A	369	182.919	168.982	-16.263	1.00	25.61	A
35	ATOM O	2031	OG	SER A	369	183.115	170.391	-16.341	1.00	37.93	A
	ATOM C	2032	C	SER A	369	182.809	166.986	-14.785	1.00	23.28	A
	ATOM O	2033	O	SER A	369	181.685	166.555	-14.591	1.00	26.91	A
40	ATOM N	2034	N	GLN A	370	183.848	166.196	-14.995	1.00	20.71	A
	ATOM C	2035	CA	GLN A	370	183.744	164.749	-15.009	1.00	21.53	A
45	ATOM C	2036	CB	GLN A	370	184.922	164.172	-15.785	1.00	24.23	A
	ATOM C	2037	CG	GLN A	370	184.674	164.178	-17.279	1.00	31.18	A
50	ATOM C	2038	CD	GLN A	370	185.948	164.183	-18.045	1.00	38.83	A
	ATOM O	2039	OE1	GLN A	370	186.879	163.380	-17.767	1.00	41.58	A
	ATOM N	2040	NE2	GLN A	370	186.033	165.098	-19.038	1.00	43.83	A
55	ATOM C	2041	C	GLN A	370	183.688	164.073	-13.665	1.00	20.69	A
	ATOM O	2042	O	GLN A	370	183.444	162.864	-13.600	1.00	19.42	A
60	ATOM N	2043	N	ARG A	371	183.940	164.804	-12.585	1.00	18.88	A
	ATOM C	2044	CA	ARG A	371	183.906	164.189	-11.252	1.00	21.24	A
	ATOM C	2045	CB	ARG A	371	184.612	165.072	-10.231	1.00	17.55	A

5	ATOM C	2046	CG	ARG A 371	186.104	165.158	-10.394	1.00	15.36	A
	ATOM C	2047	CD	ARG A 371	186.643	166.286	-9.564	1.00	11.86	A
	ATOM N	2048	NE	ARG A 371	187.913	166.739	-10.108	1.00	12.57	A
	ATOM C	2049	CZ	ARG A 371	188.440	167.951	-9.938	1.00	14.14	A
10	ATOM N	2050	NH1	ARG A 371	187.817	168.878	-9.216	1.00	10.91	A
	ATOM N	2051	NH2	ARG A 371	189.583	168.257	-10.545	1.00	9.48	A
15	ATOM C	2052	C	ARG A 371	182.440	164.038	-10.854	1.00	22.37	A
	ATOM O	2053	O	ARG A 371	181.601	164.841	-11.176	1.00	22.50	A
20	ATOM N	2054	N	PRO A 372	182.141	162.957	-10.111	1.00	23.64	A
	ATOM C	2055	CD	PRO A 372	183.165	162.051	-9.512	1.00	23.75	A
	ATOM C	2056	CA	PRO A 372	180.757	162.663	-9.653	1.00	21.80	A
25	ATOM C	2057	CB	PRO A 372	180.923	161.269	-9.007	1.00	22.29	A
	ATOM C	2058	CG	PRO A 372	182.365	161.227	-8.548	1.00	22.92	A
	ATOM C	2059	C	PRO A 372	180.160	163.726	-8.739	1.00	21.72	A
30	ATOM O	2060	O	PRO A 372	180.875	164.579	-8.217	1.00	23.11	A
	ATOM N	2061	N	MET A 373	178.840	163.740	-8.654	1.00	20.67	A
35	ATOM C	2062	CA	MET A 373	178.153	164.668	-7.731	1.00	19.68	A
	ATOM C	2063	CB	MET A 373	176.674	164.841	-8.137	1.00	25.32	A
	ATOM C	2064	CG	MET A 373	176.470	165.598	-9.397	1.00	29.58	A
40	ATOM S	2065	SD	MET A 373	177.274	167.224	-9.216	1.00	44.08	A
	ATOM C	2066	CE	MET A 373	175.850	168.314	-8.571	1.00	34.35	A
45	ATOM C	2067	C	MET A 373	178.231	163.942	-6.368	1.00	18.77	A
	ATOM O	2068	O	MET A 373	178.518	162.750	-6.337	1.00	14.31	A
	ATOM N	2069	N	LEU A 374	177.985	164.639	-5.257	1.00	16.82	A
50	ATOM C	2070	CA	LEU A 374	178.041	163.984	-3.959	1.00	17.05	A
	ATOM C	2071	CB	LEU A 374	177.959	165.010	-2.820	1.00	15.61	A
55	ATOM C	2072	CG	LEU A 374	179.224	165.888	-2.751	1.00	17.98	A
	ATOM C	2073	CD1	LEU A 374	178.940	167.269	-2.145	1.00	8.94	A
60	ATOM C	2074	CD2	LEU A 374	180.290	165.125	-1.973	1.00	12.26	A
	ATOM C	2075	C	LEU A 374	176.934	162.915	-3.837	1.00	18.65	A
	ATOM O	2076	O	LEU A 374	177.122	161.885	-3.201	1.00	19.21	A

5	ATOM N	2077	N	ARG A 375	175.804	163.167	-4.504	1.00	18.78	A
	ATOM C	2078	CA	ARG A 375	174.657	162.248	-4.510	1.00	20.13	A
	ATOM C	2079	CB	ARG A 375	173.504	162.813	-5.210	1.00	21.87	A
	ATOM C	2080	C	ARG A 375	175.033	160.942	-5.178	1.00	21.00	A
10	ATOM O	2081	O	ARG A 375	174.457	159.916	-4.909	1.00	21.05	A
	ATOM N	2082	N	GLU A 376	175.970	161.009	-6.106	1.00	23.11	A
15	ATOM C	2083	CA	GLU A 376	176.419	159.788	-6.763	1.00	23.55	A
	ATOM C	2084	CB	GLU A 376	177.142	160.139	-8.053	1.00	24.82	A
	ATOM C	2085	CG	GLU A 376	176.400	161.110	-8.977	1.00	32.25	A
20	ATOM C	2086	CD	GLU A 376	177.239	161.561	-10.206	1.00	34.95	A
	ATOM O	2087	OE1	GLU A 376	177.030	162.670	-10.770	1.00	37.06	A
25	ATOM O	2088	OE2	GLU A 376	178.110	160.783	-10.630	1.00	37.87	A
	ATOM C	2089	C	GLU A 376	177.380	158.962	-5.852	1.00	23.36	A
	ATOM O	2090	O	GLU A 376	177.448	157.712	-5.874	1.00	25.32	A
30	ATOM N	2091	N	VAL A 377	178.204	159.683	-5.113	1.00	20.65	A
	ATOM C	2092	CA	VAL A 377	179.168	159.065	-4.241	1.00	19.06	A
35	ATOM C	2093	CB	VAL A 377	180.021	160.117	-3.550	1.00	20.25	A
	ATOM C	2094	CG1	VAL A 377	180.772	159.513	-2.415	1.00	14.07	A
	ATOM C	2095	CG2	VAL A 377	180.949	160.762	-4.587	1.00	16.78	A
40	ATOM C	2096	C	VAL A 377	178.386	158.284	-3.229	1.00	20.23	A
	ATOM O	2097	O	VAL A 377	178.647	157.099	-3.037	1.00	20.59	A
45	ATOM N	2098	N	LEU A 378	177.392	158.937	-2.620	1.00	20.07	A
	ATOM C	2099	CA	LEU A 378	176.526	158.314	-1.619	1.00	20.48	A
	ATOM C	2100	CB	LEU A 378	175.514	159.346	-1.107	1.00	19.33	A
50	ATOM C	2101	CG	LEU A 378	175.794	160.087	0.237	1.00	25.33	A
	ATOM C	2102	CD1	LEU A 378	177.197	159.794	0.722	1.00	23.60	A
55	ATOM C	2103	CD2	LEU A 378	175.575	161.610	0.073	1.00	20.05	A
	ATOM C	2104	C	LEU A 378	175.812	157.030	-2.120	1.00	22.64	A
	ATOM O	2105	O	LEU A 378	175.497	156.130	-1.318	1.00	21.93	A
60	ATOM N	2106	N	GLU A 379	175.612	156.930	-3.435	1.00	19.85	A
	ATOM C	2107	CA	GLU A 379	174.972	155.756	-4.020	1.00	24.21	A

5	ATOM C	2108	CB	GLU A	379	174.038	156.118	-5.171	1.00	29.18	A
	ATOM C	2109	CG	GLU A	379	173.003	157.140	-4.872	1.00	37.87	A
10	ATOM C	2110	CD	GLU A	379	172.172	157.458	-6.104	1.00	44.63	A
	ATOM O	2111	OE1	GLU A	379	172.774	157.586	-7.214	1.00	47.26	A
15	ATOM O	2112	OE2	GLU A	379	170.924	157.587	-5.961	1.00	46.30	A
	ATOM C	2113	C	GLU A	379	175.989	154.817	-4.623	1.00	22.35	A
20	ATOM O	2114	O	GLU A	379	175.607	153.788	-5.180	1.00	22.07	A
	ATOM N	2115	N	HIS A	380	177.268	155.165	-4.555	1.00	20.53	A
25	ATOM C	2116	CA	HIS A	380	178.278	154.301	-5.145	1.00	20.63	A
	ATOM C	2117	CB	HIS A	380	179.683	154.909	-4.995	1.00	15.41	A
30	ATOM C	2118	CG	HIS A	380	180.717	154.184	-5.800	1.00	17.05	A
	ATOM C	2119	CD2	HIS A	380	181.309	154.493	-6.982	1.00	16.91	A
35	ATOM N	2120	ND1	HIS A	380	181.129	152.901	-5.498	1.00	16.78	A
	ATOM C	2121	CE1	HIS A	380	181.918	152.453	-6.459	1.00	16.66	A
40	ATOM N	2122	NE2	HIS A	380	182.042	153.399	-7.372	1.00	15.37	A
	ATOM C	2123	C	HIS A	380	178.209	152.904	-4.509	1.00	20.19	A
45	ATOM O	2124	O	HIS A	380	178.129	152.774	-3.293	1.00	21.40	A
	ATOM N	2125	N	PRO A	381	178.231	151.843	-5.333	1.00	21.11	A
50	ATOM C	2126	CD	PRO A	381	178.446	151.912	-6.792	1.00	20.62	A
	ATOM C	2127	CA	PRO A	381	178.165	150.440	-4.874	1.00	22.07	A
55	ATOM C	2128	CB	PRO A	381	178.512	149.635	-6.139	1.00	23.24	A
	ATOM C	2129	CG	PRO A	381	177.998	150.510	-7.246	1.00	25.34	A
60	ATOM C	2130	C	PRO A	381	179.103	150.109	-3.708	1.00	20.71	A
	ATOM O	2131	O	PRO A	381	178.722	149.416	-2.762	1.00	22.12	A
65	ATOM N	2132	N	TRP A	382	180.330	150.607	-3.783	1.00	19.08	A
	ATOM C	2133	CA	TRP A	382	181.307	150.367	-2.733	1.00	18.09	A
70	ATOM C	2134	CB	TRP A	382	182.667	150.885	-3.160	1.00	16.26	A
	ATOM C	2135	CG	TRP A	382	183.757	150.595	-2.180	1.00	17.75	A
75	ATOM C	2136	CD2	TRP A	382	184.370	151.524	-1.271	1.00	17.24	A
	ATOM C	2137	CE2	TRP A	382	185.366	150.816	-0.559	1.00	16.47	A
	ATOM C	2138	CE3	TRP A	382	184.165	152.882	-0.983	1.00	17.55	A

5	ATOM C	2139	CD1	TRP	A	382	184.389	149.398	-1.986	1.00	14.76	A
	ATOM N	2140	NE1	TRP	A	382	185.358	149.524	-1.022	1.00	16.65	A
	ATOM C	2141	CZ2	TRP	A	382	186.168	151.422	0.421	1.00	15.85	A
	ATOM C	2142	CZ3	TRP	A	382	184.965	153.487	-0.002	1.00	19.06	A
10	ATOM C	2143	CH2	TRP	A	382	185.951	152.754	0.687	1.00	17.35	A
	ATOM C	2144	C	TRP	A	382	180.898	151.042	-1.431	1.00	18.11	A
15	ATOM O	2145	O	TRP	A	382	181.045	150.467	-0.352	1.00	19.08	A
	ATOM N	2146	N	ILE	A	383	180.391	152.266	-1.533	1.00	18.03	A
	ATOM C	2147	CA	ILE	A	383	179.963	153.003	-0.354	1.00	17.34	A
20	ATOM C	2148	CB	ILE	A	383	179.585	154.460	-0.709	1.00	15.70	A
	ATOM C	2149	CG2	ILE	A	383	178.985	155.178	0.495	1.00	13.48	A
25	ATOM C	2150	CG1	ILE	A	383	180.841	155.212	-1.132	1.00	8.79	A
	ATOM C	2151	CD1	ILE	A	383	181.809	155.455	0.019	1.00	11.19	A
	ATOM C	2152	C	ILE	A	383	178.790	152.312	0.324	1.00	19.72	A
30	ATOM O	2153	O	ILE	A	383	178.851	152.044	1.523	1.00	21.11	A
	ATOM N	2154	N	THR	A	384	177.739	151.994	-0.428	1.00	18.67	A
35	ATOM C	2155	CA	THR	A	384	176.585	151.336	0.180	1.00	21.04	A
	ATOM C	2156	CB	THR	A	384	175.352	151.287	-0.784	1.00	22.27	A
	ATOM O	2157	OG1	THR	A	384	175.657	150.457	-1.912	1.00	23.10	A
40	ATOM C	2158	CG2	THR	A	384	174.969	152.706	-1.271	1.00	15.14	A
	ATOM C	2159	C	THR	A	384	176.868	149.921	0.721	1.00	20.77	A
45	ATOM O	2160	O	THR	A	384	176.220	149.496	1.683	1.00	24.40	A
	ATOM N	2161	N	ALA	A	385	177.835	149.206	0.138	1.00	18.85	A
	ATOM C	2162	CA	ALA	A	385	178.195	147.848	0.598	1.00	16.58	A
50	ATOM C	2163	CB	ALA	A	385	178.996	147.119	-0.481	1.00	8.89	A
	ATOM C	2164	C	ALA	A	385	179.021	147.877	1.890	1.00	19.30	A
55	ATOM O	2165	O	ALA	A	385	178.987	146.950	2.699	1.00	17.69	A
	ATOM N	2166	N	ASN	A	386	179.748	148.966	2.104	1.00	23.78	A
	ATOM C	2167	CA	ASN	A	386	180.614	149.059	3.274	1.00	24.44	A
60	ATOM C	2168	CB	ASN	A	386	182.039	149.240	2.783	1.00	22.82	A
	ATOM C	2169	CG	ASN	A	386	182.509	148.051	1.997	1.00	22.92	A

5	ATOM O	2170	OD1	ASN	A	386	182.581	146.947	2.539	1.00	23.56	A
	ATOM N	2171	ND2	ASN	A	386	182.807	148.251	0.706	1.00	20.68	A
	ATOM C	2172	C	ASN	A	386	180.305	150.133	4.291	1.00	25.32	A
	ATOM O	2173	O	ASN	A	386	180.891	150.175	5.366	1.00	25.70	A
10	ATOM N	2174	N	SER	A	387	179.385	151.009	3.950	1.00	28.67	A
	ATOM C	2175	CA	SER	A	387	179.063	152.111	4.823	1.00	30.65	A
15	ATOM C	2176	CB	SER	A	387	178.507	153.232	3.955	1.00	29.51	A
	ATOM O	2177	OG	SER	A	387	178.208	154.364	4.724	1.00	35.78	A
20	ATOM C	2178	C	SER	A	387	178.063	151.687	5.890	1.00	32.67	A
	ATOM O	2179	O	SER	A	387	177.162	150.889	5.535	1.00	35.02	A
25	ATOM O	2180	OXT	SER	A	387	178.173	152.164	7.055	1.00	35.90	A
	ATOM C	2181	CB	SER	B	7	187.273	195.899	10.921	1.00	30.72	B
30	ATOM O	2182	OG	SER	B	7	185.919	195.490	11.062	1.00	28.92	B
	ATOM C	2183	C	SER	B	7	187.728	193.792	12.227	1.00	32.69	B
35	ATOM O	2184	O	SER	B	7	187.932	192.918	11.331	1.00	33.35	B
	ATOM N	2185	N	SER	B	7	189.583	195.368	11.576	1.00	34.34	B
40	ATOM C	2186	CA	SER	B	7	188.150	195.268	12.001	1.00	32.37	B
	ATOM N	2187	N	TYR	B	8	187.139	193.527	13.402	1.00	28.10	B
45	ATOM C	2188	CA	TYR	B	8	186.671	192.188	13.775	1.00	25.10	B
	ATOM C	2189	CB	TYR	B	8	187.465	191.681	14.999	1.00	22.64	B
50	ATOM C	2190	CG	TYR	B	8	188.962	191.579	14.731	1.00	22.03	B
	ATOM C	2191	CD1	TYR	B	8	189.806	192.667	14.982	1.00	19.79	B
55	ATOM C	2192	CE1	TYR	B	8	191.153	192.623	14.642	1.00	19.33	B
	ATOM C	2193	CD2	TYR	B	8	189.524	190.435	14.128	1.00	18.09	B
60	ATOM C	2194	CE2	TYR	B	8	190.881	190.391	13.775	1.00	18.91	B
	ATOM C	2195	CZ	TYR	B	8	191.686	191.488	14.038	1.00	20.94	B
65	ATOM O	2196	OH	TYR	B	8	193.020	191.444	13.712	1.00	23.31	B
	ATOM C	2197	C	TYR	B	8	185.151	192.143	14.045	1.00	24.33	B
70	ATOM O	2198	O	TYR	B	8	184.677	191.422	14.936	1.00	23.49	B
	ATOM N	2199	N	SER	B	9	184.410	192.931	13.263	1.00	24.49	B
75	ATOM C	2200	CA	SER	B	9	182.945	193.017	13.314	1.00	24.46	B

5	ATOM C	2201	CB	SER	B	9	182.455	194.444	13.006	1.00	23.56	B
	ATOM O	2202	OG	SER	B	9	182.756	195.336	14.059	1.00	29.98	B
	ATOM C	2203	C	SER	B	9	182.426	192.085	12.229	1.00	22.36	B
	ATOM O	2204	O	SER	B	9	182.469	192.408	11.035	1.00	22.10	B
10	ATOM N	2205	N	TYR	B	10	181.926	190.938	12.653	1.00	20.97	B
	ATOM C	2206	CA	TYR	B	10	181.434	189.932	11.728	1.00	21.80	B
15	ATOM C	2207	CB	TYR	B	10	182.099	188.582	12.063	1.00	21.23	B
	ATOM C	2208	CG	TYR	B	10	183.618	188.617	12.082	1.00	23.30	B
	ATOM C	2209	CD1	TYR	B	10	184.345	187.694	12.836	1.00	24.95	B
20	ATOM C	2210	CE1	TYR	B	10	185.744	187.683	12.816	1.00	25.40	B
	ATOM C	2211	CD2	TYR	B	10	184.331	189.542	11.311	1.00	23.55	B
25	ATOM C	2212	CE2	TYR	B	10	185.725	189.541	11.285	1.00	24.34	B
	ATOM C	2213	CZ	TYR	B	10	186.421	188.600	12.036	1.00	26.19	B
	ATOM O	2214	OH	TYR	B	10	187.800	188.526	11.956	1.00	31.92	B
30	ATOM C	2215	C	TYR	B	10	179.918	189.807	11.832	1.00	21.84	B
	ATOM O	2216	O	TYR	B	10	179.334	190.098	12.872	1.00	22.91	B
35	ATOM N	2217	N	ASP	B	11	179.283	189.372	10.754	1.00	19.80	B
	ATOM C	2218	CA	ASP	B	11	177.842	189.173	10.751	1.00	19.63	B
	ATOM C	2219	CB	ASP	B	11	177.308	189.274	9.310	1.00	21.09	B
40	ATOM C	2220	CG	ASP	B	11	175.778	189.141	9.217	1.00	23.91	B
	ATOM O	2221	OD1	ASP	B	11	175.093	188.957	10.256	1.00	24.67	B
45	ATOM O	2222	OD2	ASP	B	11	175.264	189.221	8.077	1.00	22.90	B
	ATOM C	2223	C	ASP	B	11	177.653	187.756	11.297	1.00	19.67	B
	ATOM O	2224	O	ASP	B	11	177.383	186.820	10.565	1.00	20.37	B
50	ATOM N	2225	N	ALA	B	12	177.844	187.593	12.590	1.00	19.26	B
	ATOM C	2226	CA	ALA	B	12	177.696	186.285	13.174	1.00	19.72	B
55	ATOM C	2227	CB	ALA	B	12	178.993	185.498	13.013	1.00	20.60	B
	ATOM C	2228	C	ALA	B	12	177.337	186.502	14.640	1.00	20.60	B
	ATOM O	2229	O	ALA	B	12	177.450	187.632	15.149	1.00	20.41	B
60	ATOM N	2230	N	PRO	B	13	176.918	185.448	15.350	1.00	20.13	B
	ATOM C	2231	CD	PRO	B	13	176.769	184.055	14.907	1.00	17.56	B



5	ATOM C	2263	CA	ILE	B	17	173.652	182.163	25.182	1.00	20.86	B
	ATOM C	2264	CB	ILE	B	17	173.965	181.144	24.009	1.00	21.47	B
	ATOM C	2265	CG2	ILE	B	17	172.988	179.964	24.011	1.00	11.76	B
	ATOM C	2266	CG1	ILE	B	17	173.957	181.844	22.654	1.00	16.04	B
10	ATOM C	2267	CD1	ILE	B	17	174.760	181.051	21.631	1.00	18.42	B
	ATOM C	2268	C	ILE	B	17	173.478	181.318	26.439	1.00	21.56	B
15	ATOM O	2269	O	ILE	B	17	174.462	180.965	27.086	1.00	23.11	B
	ATOM N	2270	N	ASN	B	18	172.227	181.002	26.778	1.00	24.87	B
	ATOM C	2271	CA	ASN	B	18	171.893	180.143	27.928	1.00	26.79	B
20	ATOM C	2272	CB	ASN	B	18	170.485	180.437	28.427	1.00	26.34	B
	ATOM C	2273	CG	ASN	B	18	170.052	179.482	29.543	1.00	30.28	B
25	ATOM O	2274	OD1	ASN	B	18	170.753	178.519	29.870	1.00	30.01	B
	ATOM N	2275	ND2	ASN	B	18	168.893	179.747	30.125	1.00	28.50	B
	ATOM C	2276	C	ASN	B	18	171.911	178.718	27.373	1.00	28.06	B
30	ATOM O	2277	O	ASN	B	18	170.947	178.305	26.737	1.00	31.09	B
	ATOM N	2278	N	PHE	B	19	172.969	177.950	27.616	1.00	30.32	B
35	ATOM C	2279	CA	PHE	B	19	173.027	176.599	27.050	1.00	32.46	B
	ATOM C	2280	CB	PHE	B	19	174.460	176.061	27.076	1.00	27.50	B
	ATOM C	2281	CG	PHE	B	19	175.430	176.837	26.214	1.00	22.59	B
40	ATOM C	2282	CD1	PHE	B	19	176.332	177.737	26.785	1.00	20.42	B
	ATOM C	2283	CD2	PHE	B	19	175.426	176.682	24.831	1.00	21.89	B
45	ATOM C	2284	CE1	PHE	B	19	177.223	178.454	25.989	1.00	19.77	B
	ATOM C	2285	CE2	PHE	B	19	176.312	177.398	24.021	1.00	18.13	B
	ATOM C	2286	CZ	PHE	B	19	177.206	178.291	24.605	1.00	19.50	B
50	ATOM C	2287	C	PHE	B	19	172.086	175.529	27.618	1.00	36.90	B
	ATOM O	2288	O	PHE	B	19	172.063	174.397	27.124	1.00	41.31	B
55	ATOM N	2289	N	SER	B	20	171.317	175.844	28.646	1.00	41.32	B
	ATOM C	2290	CA	SER	B	20	170.402	174.824	29.142	1.00	46.46	B
	ATOM C	2291	CB	SER	B	20	170.317	174.921	30.652	1.00	47.60	B
60	ATOM O	2292	OG	SER	B	20	170.456	176.275	31.032	1.00	49.62	B
	ATOM C	2293	C	SER	B	20	169.029	175.021	28.496	1.00	48.43	B

5	ATOM O	2294	O	SER	B	20	168.337	174.060	28.170	1.00	50.43	B
	ATOM N	2295	N	SER	B	21	168.645	176.275	28.286	1.00	50.08	B
	ATOM C	2296	CA	SER	B	21	167.349	176.574	27.676	1.00	50.65	B
	ATOM C	2297	CB	SER	B	21	166.742	177.810	28.317	1.00	49.82	B
10	ATOM O	2298	OG	SER	B	21	167.467	178.945	27.866	1.00	50.01	B
	ATOM C	2299	C	SER	B	21	167.581	176.880	26.204	1.00	51.89	B
15	ATOM O	2300	O	SER	B	21	166.843	176.336	25.325	1.00	51.53	B
	ATOM O	2301	OXT	SER	B	21	168.482	177.716	25.953	1.00	53.54	B
20	ATOM C	2302	CB	ASN	C	30	165.336	177.781	10.155	1.00	41.18	C
	ATOM C	2303	CG	ASN	C	30	164.486	178.568	9.178	1.00	46.58	C
	ATOM O	2304	OD1	ASN	C	30	164.828	179.693	8.808	1.00	49.62	C
	ATOM N	2305	ND2	ASN	C	30	163.363	177.973	8.740	1.00	49.11	C
25	ATOM C	2306	C	ASN	C	30	167.301	179.381	10.314	1.00	36.00	C
	ATOM O	2307	O	ASN	C	30	167.202	179.731	9.143	1.00	34.36	C
30	ATOM N	2308	N	ASN	C	30	165.267	179.744	11.676	1.00	37.72	C
	ATOM C	2309	CA	ASN	C	30	166.154	178.688	11.078	1.00	38.33	C
35	ATOM N	2310	N	ILE	C	31	168.406	179.537	11.026	1.00	32.89	C
	ATOM C	2311	CA	ILE	C	31	169.605	180.229	10.589	1.00	28.57	C
	ATOM C	2312	CB	ILE	C	31	170.635	180.011	11.676	1.00	31.08	C
40	ATOM C	2313	CG2	ILE	C	31	171.873	180.840	11.426	1.00	30.71	C
	ATOM C	2314	CG1	ILE	C	31	169.991	180.405	13.012	1.00	34.10	C
	ATOM C	2315	CD1	ILE	C	31	169.738	181.909	13.147	1.00	41.37	C
45	ATOM C	2316	C	ILE	C	31	170.254	180.041	9.214	1.00	25.67	C
	ATOM O	2317	O	ILE	C	31	170.816	180.996	8.677	1.00	20.90	C
50	ATOM N	2318	N	ASP	C	32	170.188	178.856	8.623	1.00	23.52	C
	ATOM C	2319	CA	ASP	C	32	170.872	178.678	7.351	1.00	24.02	C
	ATOM C	2320	CB	ASP	C	32	171.126	177.197	7.086	1.00	27.28	C
55	ATOM C	2321	CG	ASP	C	32	169.858	176.423	6.805	1.00	32.74	C
	ATOM O	2322	OD1	ASP	C	32	168.852	177.009	6.338	1.00	36.15	C
60	ATOM O	2323	OD2	ASP	C	32	169.884	175.202	7.039	1.00	33.71	C
	ATOM C	2324	C	ASP	C	32	170.289	179.324	6.104	1.00	23.19	C

5	ATOM O	2325	O	ASP	C	32	170.804	179.126	5.001	1.00	22.55	C
	ATOM N	2326	N	SER	C	33	169.223	180.090	6.271	1.00	21.46	C
	ATOM C	2327	CA	SER	C	33	168.608	180.781	5.136	1.00	22.57	C
	ATOM C	2328	CB	SER	C	33	167.205	181.244	5.499	1.00	23.28	C
10	ATOM O	2329	OG	SER	C	33	166.326	180.142	5.639	1.00	33.59	C
	ATOM C	2330	C	SER	C	33	169.448	182.002	4.805	1.00	19.49	C
15	ATOM O	2331	O	SER	C	33	169.273	182.639	3.770	1.00	20.33	C
	ATOM N	2332	N	TRP	C	34	170.344	182.330	5.728	1.00	18.04	C
20	ATOM C	2333	CA	TRP	C	34	171.254	183.466	5.621	1.00	16.02	C
	ATOM C	2334	CB	TRP	C	34	172.234	183.422	6.792	1.00	15.82	C
	ATOM C	2335	CG	TRP	C	34	173.240	184.531	6.836	1.00	15.40	C
	ATOM C	2336	CD2	TRP	C	34	174.599	184.462	6.404	1.00	13.15	C
25	ATOM C	2337	CE2	TRP	C	34	175.180	185.735	6.640	1.00	14.42	C
	ATOM C	2338	CE3	TRP	C	34	175.387	183.451	5.843	1.00	10.87	C
30	ATOM C	2339	CD1	TRP	C	34	173.052	185.801	7.302	1.00	13.49	C
	ATOM N	2340	NE1	TRP	C	34	174.212	186.530	7.189	1.00	11.42	C
35	ATOM C	2341	CZ2	TRP	C	34	176.523	186.024	6.330	1.00	14.91	C
	ATOM C	2342	CZ3	TRP	C	34	176.727	183.738	5.538	1.00	12.26	C
	ATOM C	2343	CH2	TRP	C	34	177.278	185.016	5.785	1.00	10.61	C
	ATOM C	2344	C	TRP	C	34	172.022	183.499	4.299	1.00	15.62	C
40	ATOM O	2345	O	TRP	C	34	172.251	184.579	3.735	1.00	16.88	C
	ATOM N	2346	N	PHE	C	35	172.435	182.324	3.819	1.00	13.45	C
45	ATOM C	2347	CA	PHE	C	35	173.191	182.222	2.567	1.00	12.33	C
	ATOM C	2348	CB	PHE	C	35	173.739	180.801	2.344	1.00	8.78	C
50	ATOM C	2349	CG	PHE	C	35	174.597	180.304	3.456	1.00	9.30	C
	ATOM C	2350	CD1	PHE	C	35	174.042	179.566	4.495	1.00	9.43	C
55	ATOM C	2351	CD2	PHE	C	35	175.960	180.610	3.500	1.00	9.38	C
	ATOM C	2352	CE1	PHE	C	35	174.822	179.141	5.565	1.00	6.69	C
60	ATOM C	2353	CE2	PHE	C	35	176.749	180.190	4.569	1.00	8.62	C
	ATOM C	2354	CZ	PHE	C	35	176.174	179.455	5.602	1.00	10.55	C
	ATOM C	2355	C	PHE	C	35	172.367	182.623	1.351	1.00	13.51	C

5	ATOM O	2356	O	PHE	C	35	172.779	183.502	0.597	1.00	13.63	C
	ATOM N	2357	N	ALA	C	36	171.207	181.997	1.153	1.00	14.52	C
	ATOM C	2358	CA	ALA	C	36	170.392	182.349	-0.008	1.00	18.05	C
	ATOM C	2359	CB	ALA	C	36	169.246	181.349	-0.209	1.00	13.28	C
	ATOM C	2360	C	ALA	C	36	169.844	183.775	0.103	1.00	18.08	C
10	ATOM O	2361	O	ALA	C	36	169.797	184.500	-0.899	1.00	20.25	C
	ATOM N	2362	N	GLU	C	37	169.458	184.192	1.307	1.00	18.61	C
15	ATOM C	2363	CA	GLU	C	37	168.905	185.536	1.505	1.00	21.91	C
	ATOM C	2364	CB	GLU	C	37	168.391	185.686	2.933	1.00	22.41	C
20	ATOM C	2365	CG	GLU	C	37	167.103	184.901	3.240	1.00	24.75	C
	ATOM C	2366	CD	GLU	C	37	166.619	185.133	4.681	1.00	30.55	C
25	ATOM O	2367	OE1	GLU	C	37	167.473	185.511	5.529	1.00	31.00	C
	ATOM O	2368	OE2	GLU	C	37	165.414	184.932	4.976	1.00	30.11	C
30	ATOM C	2369	C	GLU	C	37	169.913	186.649	1.194	1.00	22.74	C
	ATOM O	2370	O	GLU	C	37	169.561	187.754	0.791	1.00	22.40	C
35	ATOM N	2371	N	LYS	C	38	171.181	186.332	1.375	1.00	25.80	C
	ATOM C	2372	CA	LYS	C	38	172.269	187.252	1.114	1.00	24.79	C
40	ATOM C	2373	CB	LYS	C	38	173.438	186.831	1.982	1.00	27.15	C
	ATOM C	2374	CG	LYS	C	38	174.708	187.488	1.649	1.00	30.16	C
45	ATOM C	2375	CD	LYS	C	38	175.776	187.057	2.622	1.00	31.96	C
	ATOM C	2376	CE	LYS	C	38	177.007	187.927	2.391	1.00	35.28	C
50	ATOM N	2377	NZ	LYS	C	38	178.028	187.735	3.456	1.00	40.31	C
	ATOM C	2378	C	LYS	C	38	172.625	187.194	-0.373	1.00	25.05	C
55	ATOM O	2379	O	LYS	C	38	173.062	188.177	-0.969	1.00	23.54	C
	ATOM N	2380	N	ALA	C	39	172.418	186.032	-0.975	1.00	23.76	C
60	ATOM C	2381	CA	ALA	C	39	172.687	185.849	-2.400	1.00	23.35	C
	ATOM C	2382	CB	ALA	C	39	172.656	184.343	-2.762	1.00	20.98	C
65	ATOM C	2383	C	ALA	C	39	171.642	186.576	-3.245	1.00	24.77	C
	ATOM O	2384	O	ALA	C	39	171.950	187.112	-4.318	1.00	24.28	C
70	ATOM N	2385	N	ASN	C	40	170.403	186.592	-2.754	1.00	23.38	C
	ATOM C	2386	CA	ASN	C	40	169.306	187.210	-3.480	1.00	23.68	C

5	ATOM C	2387	CB	ASN	C	40	167.993	186.526	-3.137	1.00	18.03	C
	ATOM C	2388	CG	ASN	C	40	168.024	185.035	-3.395	1.00	17.89	C
	ATOM O	2389	OD1	ASN	C	40	168.646	184.553	-4.351	1.00	18.06	C
	ATOM N	2390	ND2	ASN	C	40	167.325	184.287	-2.545	1.00	16.76	C
10	ATOM C	2391	C	ASN	C	40	169.122	188.701	-3.279	1.00	25.17	C
	ATOM O	2392	O	ASN	C	40	168.413	189.332	-4.052	1.00	27.11	C
15	ATOM N	2393	N	LEU	C	41	169.731	189.268	-2.246	1.00	26.95	C
	ATOM C	2394	CA	LEU	C	41	169.600	190.709	-1.965	1.00	29.31	C
20	ATOM C	2395	CB	LEU	C	41	170.380	191.047	-0.705	1.00	29.88	C
	ATOM C	2396	CG	LEU	C	41	169.816	192.308	-0.057	1.00	30.53	C
	ATOM C	2397	CD1	LEU	C	41	168.319	192.148	0.221	1.00	30.41	C
25	ATOM C	2398	CD2	LEU	C	41	170.580	192.558	1.209	1.00	29.64	C
	ATOM C	2399	C	LEU	C	41	170.091	191.589	-3.120	1.00	29.84	C
	ATOM O	2400	O	LEU	C	41	171.051	191.230	-3.787	1.00	30.13	C
30	ATOM N	2401	N	GLU	C	42	169.487	192.763	-3.312	1.00	32.17	C
	ATOM C	2402	CA	GLU	C	42	169.851	193.627	-4.439	1.00	35.33	C
35	ATOM C	2403	CB	GLU	C	42	168.583	193.847	-5.286	1.00	33.50	C
	ATOM C	2404	CG	GLU	C	42	167.819	192.560	-5.616	1.00	32.30	C
	ATOM C	2405	CD	GLU	C	42	166.473	192.784	-6.334	1.00	34.80	C
40	ATOM O	2406	OE1	GLU	C	42	165.892	193.892	-6.241	1.00	34.22	C
	ATOM O	2407	OE2	GLU	C	42	165.980	191.829	-6.987	1.00	33.99	C
45	ATOM C	2408	C	GLU	C	42	170.537	194.977	-4.190	1.00	37.36	C
	ATOM O	2409	O	GLU	C	42	170.487	195.539	-3.109	1.00	38.22	C
	ATOM N	2410	N	ASN	C	43	171.220	195.457	-5.221	1.00	43.15	C
50	ATOM C	2411	CA	ASN	C	43	171.863	196.790	-5.266	1.00	48.74	C
	ATOM C	2412	CB	ASN	C	43	172.611	197.184	-3.967	1.00	48.84	C
55	ATOM C	2413	CG	ASN	C	43	173.769	196.255	-3.632	1.00	50.97	C
	ATOM O	2414	OD1	ASN	C	43	173.749	195.054	-3.970	1.00	50.34	C
	ATOM N	2415	ND2	ASN	C	43	174.793	196.804	-2.939	1.00	51.10	C
60	ATOM C	2416	C	ASN	C	43	172.809	196.704	-6.455	1.00	52.67	C
	ATOM O	2417	O	ASN	C	43	172.493	197.379	-7.493	1.00	54.34	C

5	ATOM O	2418	OXT	ASN	C	43	173.808	195.931	-6.344	1.00	55.98	C
	ATOM P	2419	PB	ADP	S	531	193.788	175.824	12.432	1.00	20.87	S
10	ATOM O	2420	O1B	ADP	S	531	193.884	176.352	13.792	1.00	32.28	S
	ATOM O	2421	O2B	ADP	S	531	193.566	176.837	11.394	1.00	26.12	S
15	ATOM O	2422	O3B	ADP	S	531	194.979	174.908	12.132	1.00	31.89	S
	ATOM P	2423	PA	ADP	S	531	191.748	174.063	13.545	1.00	18.35	S
20	ATOM O	2424	O1A	ADP	S	531	190.611	174.901	14.032	1.00	26.99	S
	ATOM O	2425	O2A	ADP	S	531	191.357	172.755	12.954	1.00	26.80	S
25	ATOM O	2426	O3A	ADP	S	531	192.532	174.874	12.450	1.00	28.14	S
	ATOM O	2427	O5*	ADP	S	531	192.642	173.906	14.839	1.00	22.21	S
30	ATOM C	2428	C5*	ADP	S	531	193.768	172.965	14.869	1.00	20.71	S
	ATOM C	2429	C4*	ADP	S	531	193.594	171.623	15.640	1.00	17.30	S
35	ATOM O	2430	O4*	ADP	S	531	192.923	171.842	16.897	1.00	18.08	S
	ATOM C	2431	C3*	ADP	S	531	192.751	170.494	14.997	1.00	17.80	S
40	ATOM O	2432	O3*	ADP	S	531	193.561	169.824	14.038	1.00	18.78	S
	ATOM C	2433	C2*	ADP	S	531	192.369	169.659	16.218	1.00	19.78	S
45	ATOM O	2434	O2*	ADP	S	531	193.423	168.749	16.615	1.00	19.10	S
	ATOM C	2435	C1*	ADP	S	531	192.152	170.704	17.312	1.00	18.01	S
50	ATOM N	2436	N9	ADP	S	531	190.711	171.169	17.445	1.00	18.12	S
	ATOM C	2437	C8	ADP	S	531	190.169	172.237	16.808	1.00	20.72	S
55	ATOM N	2438	N7	ADP	S	531	188.877	172.431	17.108	1.00	19.94	S
	ATOM C	2439	C5	ADP	S	531	188.596	171.408	17.961	1.00	15.87	S
60	ATOM C	2440	C6	ADP	S	531	187.377	171.071	18.652	1.00	14.49	S
	ATOM N	2441	N6	ADP	S	531	186.260	171.696	18.563	1.00	9.66	S
65	ATOM N	2442	N1	ADP	S	531	187.474	169.935	19.454	1.00	13.01	S
	ATOM C	2443	C2	ADP	S	531	188.642	169.198	19.595	1.00	14.56	S
70	ATOM N	2444	N3	ADP	S	531	189.773	169.512	18.982	1.00	17.25	S
	ATOM C	2445	C4	ADP	S	531	189.716	170.610	18.162	1.00	16.09	S
75	ATOM MG+2	2446	MG	MG	X	1	192.801	173.013	10.897	1.00	18.98	X
	ATOM MG+2	2447	MG	MG	X	2	192.933	178.461	10.215	1.00	21.17	X
	ATOM MG+2	2448	MG	MG	X	3	174.135	172.090	-6.081	1.00	37.43	X

5	ATOM S	2449	S	SO4	Y	1	175.520	167.060	-4.810	1.00	40.27	Y
	ATOM O	2450	O1	SO4	Y	1	175.005	168.134	-3.755	1.00	40.61	Y
	ATOM O	2451	O2	SO4	Y	1	176.918	167.395	-5.118	1.00	40.85	Y
	ATOM O	2452	O3	SO4	Y	1	175.333	165.874	-4.319	1.00	45.29	Y
10	ATOM O	2453	O4	SO4	Y	1	174.705	167.387	-6.003	1.00	46.53	Y
	ATOM S	2454	S	SO4	Y	2	196.317	160.442	22.149	1.00	52.91	Y
15	ATOM O	2455	O1	SO4	Y	2	194.902	160.702	22.904	1.00	53.25	Y
	ATOM O	2456	O2	SO4	Y	2	197.156	161.615	22.484	1.00	52.23	Y
	ATOM O	2457	O3	SO4	Y	2	196.808	159.261	22.506	1.00	50.45	Y
20	ATOM O	2458	O4	SO4	Y	2	195.932	160.567	20.717	1.00	53.17	Y
	ATOM S	2459	S	SO4	Y	3	184.237	187.281	-0.473	1.00	69.64	Y
25	ATOM O	2460	O1	SO4	Y	3	182.905	188.209	-0.613	1.00	70.60	Y
	ATOM O	2461	O2	SO4	Y	3	185.274	188.143	0.172	1.00	70.08	Y
	ATOM O	2462	O3	SO4	Y	3	183.925	186.181	0.170	1.00	69.68	Y
30	ATOM O	2463	O4	SO4	Y	3	184.641	187.119	-1.915	1.00	70.92	Y
	ATOM O	2464	OH2	WAT	W	1	179.030	185.642	-6.293	1.00	8.84	W
35	ATOM O	2465	OH2	WAT	W	2	194.313	179.202	-8.444	1.00	16.79	W
	ATOM O	2466	OH2	WAT	W	3	192.921	180.168	8.084	1.00	30.46	W
	ATOM O	2467	OH2	WAT	W	4	187.994	175.656	4.804	1.00	16.00	W
40	ATOM O	2468	OH2	WAT	W	5	178.455	169.305	-5.499	1.00	13.87	W
	ATOM O	2469	OH2	WAT	W	6	197.111	180.066	22.244	1.00	15.19	W
45	ATOM O	2470	OH2	WAT	W	7	180.414	171.384	22.814	1.00	8.30	W
	ATOM O	2471	OH2	WAT	W	8	188.179	184.543	-6.390	1.00	10.24	W
	ATOM O	2472	OH2	WAT	W	9	188.183	181.649	3.509	1.00	23.15	W
50	ATOM O	2473	OH2	WAT	W	10	185.065	157.114	14.496	1.00	16.39	W
	ATOM O	2474	OH2	WAT	W	11	192.854	158.543	18.441	1.00	20.42	W
55	ATOM O	2475	OH2	WAT	W	12	194.144	171.703	11.618	1.00	13.61	W
	ATOM O	2476	OH2	WAT	W	13	194.572	183.197	-8.077	1.00	36.64	W
	ATOM O	2477	OH2	WAT	W	14	198.254	147.344	-7.377	1.00	23.99	W
60	ATOM O	2478	OH2	WAT	W	15	174.141	170.073	-2.678	1.00	18.36	W
	ATOM O	2479	OH2	WAT	W	16	197.136	162.247	7.860	1.00	20.24	W

5	ATOM	2480	OH2	WAT	W	17	178.742	175.122	-2.821	1.00	12.41	W
	O											
	ATOM	2481	OH2	WAT	W	18	200.365	168.406	2.165	1.00	9.98	W
	O											
	ATOM	2482	OH2	WAT	W	19	168.522	176.594	9.704	1.00	27.47	W
10	O											
	ATOM	2483	OH2	WAT	W	20	193.215	179.995	11.973	1.00	17.15	W
	O											
	ATOM	2484	OH2	WAT	W	21	188.165	173.468	14.493	1.00	18.83	W
	O											
15	ATOM	2485	OH2	WAT	W	22	178.977	189.493	5.006	1.00	25.99	W
	O											
	ATOM	2486	OH2	WAT	W	23	194.904	178.835	14.332	1.00	9.84	W
	O											
	ATOM	2487	OH2	WAT	W	24	172.594	187.824	25.336	1.00	22.88	W
20	O											
	ATOM	2488	OH2	WAT	W	25	186.612	173.366	-9.877	1.00	19.22	W
	O											
	ATOM	2489	OH2	WAT	W	26	176.840	183.702	20.193	1.00	22.57	W
	O											
25	ATOM	2490	OH2	WAT	W	27	176.801	160.388	11.646	1.00	15.90	W
	O											
	ATOM	2491	OH2	WAT	W	28	178.487	174.788	11.702	1.00	18.10	W
	O											
	ATOM	2492	OH2	WAT	W	29	181.155	186.952	32.619	1.00	32.00	W
30	O											
	ATOM	2493	OH2	WAT	W	30	209.304	163.564	-16.281	1.00	27.44	W
	O											
	ATOM	2494	OH2	WAT	W	31	203.827	165.930	-0.838	1.00	16.37	W
	O											
35	ATOM	2495	OH2	WAT	W	32	183.937	190.638	21.333	1.00	17.02	W
	O											
	ATOM	2496	OH2	WAT	W	33	190.362	181.451	8.363	1.00	23.84	W
	O											
	ATOM	2497	OH2	WAT	W	34	201.524	183.136	11.412	1.00	27.78	W
40	O											
	ATOM	2498	OH2	WAT	W	35	176.401	172.283	12.285	1.00	22.44	W
	O											
	ATOM	2499	OH2	WAT	W	36	191.486	178.801	-8.556	1.00	14.47	W
	O											
45	ATOM	2500	OH2	WAT	W	37	193.706	178.975	16.555	1.00	28.73	W
	O											
	ATOM	2501	OH2	WAT	W	38	200.711	191.015	5.492	1.00	22.39	W
	O											
	ATOM	2502	OH2	WAT	W	39	198.698	163.980	-2.087	1.00	16.88	W
50	O											
	ATOM	2503	OH2	WAT	W	40	186.096	174.714	13.402	1.00	14.25	W
	O											
	ATOM	2504	OH2	WAT	W	41	189.561	189.228	27.405	1.00	21.42	W
	O											
55	ATOM	2505	OH2	WAT	W	42	185.742	175.020	-12.633	1.00	32.61	W
	O											
	ATOM	2506	OH2	WAT	W	43	189.284	166.218	21.436	1.00	18.57	W
	O											
	ATOM	2507	OH2	WAT	W	44	189.806	150.396	10.582	1.00	17.00	W
60	O											
	ATOM	2508	OH2	WAT	W	45	182.606	183.843	1.498	1.00	23.82	W
	O											
	ATOM	2509	OH2	WAT	W	46	203.088	159.272	-4.093	1.00	20.75	W
	O											
	ATOM	2510	OH2	WAT	W	47	197.775	190.097	18.980	1.00	22.00	W
	O											

5	ATOM	2511	OH2	WAT	W	48	193.113	164.352	18.292	1.00	18.52	W
	O											
10	ATOM	2512	OH2	WAT	W	49	188.303	192.170	8.139	1.00	29.33	W
	O											
15	ATOM	2513	OH2	WAT	W	50	178.988	188.073	29.292	1.00	22.03	W
	O											
20	ATOM	2514	OH2	WAT	W	51	179.041	176.835	-4.879	1.00	28.93	W
	O											
25	ATOM	2515	OH2	WAT	W	52	177.094	169.275	14.745	1.00	17.83	W
	O											
30	ATOM	2516	OH2	WAT	W	53	173.359	158.848	5.717	1.00	26.69	W
	O											
35	ATOM	2517	OH2	WAT	W	54	184.713	145.517	-1.099	1.00	25.66	W
	O											
40	ATOM	2518	OH2	WAT	W	55	197.989	162.673	24.709	1.00	31.35	W
	O											
45	ATOM	2519	OH2	WAT	W	56	190.279	149.132	-0.366	1.00	23.37	W
	O											
50	ATOM	2520	OH2	WAT	W	57	175.195	156.308	1.515	1.00	25.31	W
	O											
55	ATOM	2521	OH2	WAT	W	58	189.320	149.244	12.871	1.00	39.74	W
	O											
60	ATOM	2522	OH2	WAT	W	59	191.345	160.562	17.366	1.00	19.61	W
	O											
65	ATOM	2523	OH2	WAT	W	60	209.300	189.438	10.191	1.00	32.59	W
	O											
70	ATOM	2524	OH2	WAT	W	61	176.961	195.154	23.343	1.00	26.84	W
	O											
75	ATOM	2525	OH2	WAT	W	62	194.908	178.479	10.038	1.00	12.42	W
	O											
80	ATOM	2526	OH2	WAT	W	63	192.932	176.681	8.727	1.00	17.49	W
	O											
85	ATOM	2527	OH2	WAT	W	64	191.151	178.650	10.287	1.00	25.58	W
	O											
90	ATOM	2528	OH2	WAT	W	65	182.000	183.023	-13.348	1.00	15.88	W
	O											
95	ATOM	2529	OH2	WAT	W	66	174.844	179.377	29.234	1.00	21.85	W
	O											
100	ATOM	2530	OH2	WAT	W	67	192.666	150.025	4.037	1.00	24.70	W
	O											
105	ATOM	2531	OH2	WAT	W	68	191.227	167.117	19.848	1.00	27.52	W
	O											
110	ATOM	2532	OH2	WAT	W	69	195.798	166.787	-4.678	1.00	16.05	W
	O											
115	ATOM	2533	OH2	WAT	W	70	188.683	164.953	24.250	1.00	16.65	W
	O											
120	ATOM	2534	OH2	WAT	W	71	202.921	187.953	5.807	1.00	25.48	W
	O											
125	ATOM	2535	OH2	WAT	W	72	173.656	180.838	-1.296	1.00	19.16	W
	O											
130	ATOM	2536	OH2	WAT	W	73	178.223	170.722	21.753	1.00	28.96	W
	O											
135	ATOM	2537	OH2	WAT	W	74	200.047	185.273	4.691	1.00	36.63	W
	O											
140	ATOM	2538	OH2	WAT	W	75	199.421	160.492	21.694	1.00	54.41	W
	O											
145	ATOM	2539	OH2	WAT	W	76	174.343	151.575	-4.090	1.00	24.22	W
	O											
150	ATOM	2540	OH2	WAT	W	77	199.217	156.232	8.084	1.00	24.50	W
	O											
155	ATOM	2541	OH2	WAT	W	78	186.693	195.451	15.184	1.00	30.28	W
	O											

5	ATOM	2542	OH2	WAT	W	79	204.072	167.051	-16.474	1.00	30.81	W
	O											
10	ATOM	2543	OH2	WAT	W	80	189.729	170.883	13.071	1.00	24.00	W
	O											
	ATOM	2544	OH2	WAT	W	81	193.562	167.033	18.576	1.00	34.40	W
	O											
	ATOM	2545	OH2	WAT	W	82	188.055	177.150	-16.174	1.00	39.31	W
	O											
	ATOM	2546	OH2	WAT	W	83	209.167	161.801	-3.764	1.00	29.76	W
	O											
	ATOM	2547	OH2	WAT	W	84	189.954	187.203	-3.104	1.00	30.21	W
	O											
	ATOM	2548	OH2	WAT	W	85	166.356	175.210	9.226	1.00	35.64	W
	O											
15	ATOM	2549	OH2	WAT	W	86	209.038	162.643	-13.951	1.00	29.71	W
	O											
	ATOM	2550	OH2	WAT	W	87	179.913	164.861	20.417	1.00	23.03	W
	O											
20	ATOM	2551	OH2	WAT	W	88	176.985	177.272	13.711	1.00	28.39	W
	O											
	ATOM	2552	OH2	WAT	W	89	197.775	160.663	10.355	1.00	30.90	W
	O											
	ATOM	2553	OH2	WAT	W	90	180.418	156.423	-15.983	1.00	38.69	W
	O											
25	ATOM	2554	OH2	WAT	W	91	197.603	165.048	7.104	1.00	39.85	W
	O											
	ATOM	2555	OH2	WAT	W	92	201.038	146.684	-3.627	1.00	28.72	W
	O											
30	ATOM	2556	OH2	WAT	W	93	191.798	173.307	-1.526	1.00	20.55	W
	O											
	ATOM	2557	OH2	WAT	W	94	195.433	186.638	2.426	1.00	32.36	W
	O											
	ATOM	2558	OH2	WAT	W	95	185.689	149.073	10.194	1.00	32.44	W
	O											
35	ATOM	2559	OH2	WAT	W	96	181.725	186.361	4.468	1.00	44.13	W
	O											
	ATOM	2560	OH2	WAT	W	97	190.638	181.376	1.418	1.00	40.50	W
	O											
40	ATOM	2561	OH2	WAT	W	98	203.221	164.983	2.765	1.00	30.78	W
	O											
	ATOM	2562	OH2	WAT	W	99	191.430	148.459	1.931	1.00	29.87	W
	O											
	ATOM	2563	OH2	WAT	W	100	172.186	178.856	-0.480	1.00	35.57	W
	O											
45	ATOM	2564	OH2	WAT	W	101	195.541	178.234	1.979	1.00	25.17	W
	O											
	ATOM	2565	OH2	WAT	W	102	170.598	187.029	21.078	1.00	24.60	W
	O											
50	ATOM	2566	OH2	WAT	W	103	175.607	172.274	-8.036	1.00	36.47	W
	O											
	ATOM	2567	OH2	WAT	W	104	168.429	188.864	-6.367	1.00	22.94	W
	O											
	ATOM	2568	OH2	WAT	W	105	186.340	190.812	24.666	1.00	32.99	W
	O											
55	ATOM	2569	OH2	WAT	W	106	201.816	192.555	4.023	1.00	28.31	W
	O											
	ATOM	2570	OH2	WAT	W	107	202.504	159.814	-7.441	1.00	22.58	W
	O											
60	ATOM	2571	OH2	WAT	W	108	174.542	185.298	-11.131	1.00	31.96	W
	O											
	ATOM	2572	OH2	WAT	W	109	175.457	179.403	15.662	1.00	39.35	W
	O											

5	ATOM O	2573	OH2	WAT	W	110	196.564	193.700	7.818	1.00	32.38	W
	ATOM O	2574	OH2	WAT	W	111	173.232	181.808	-8.349	1.00	19.06	W
	ATOM O	2575	OH2	WAT	W	112	182.827	187.517	-4.364	1.00	45.61	W
	ATOM O	2576	OH2	WAT	W	113	189.838	194.231	7.217	1.00	42.16	W
10	ATOM O	2577	OH2	WAT	W	114	191.170	159.628	-12.340	1.00	35.35	W
	ATOM O	2578	OH2	WAT	W	115	191.207	184.866	-0.535	1.00	34.38	W
	ATOM O	2579	OH2	WAT	W	116	183.572	197.288	15.706	1.00	39.58	W
	ATOM O	2580	OH2	WAT	W	117	199.841	150.695	13.176	1.00	35.40	W
15	ATOM O	2581	OH2	WAT	W	118	174.316	180.622	18.227	1.00	29.36	W
	ATOM O	2582	OH2	WAT	W	119	174.539	169.945	15.478	1.00	36.75	W
	ATOM O	2583	OH2	WAT	W	120	186.965	189.198	27.316	1.00	33.73	W
	ATOM O	2584	OH2	WAT	W	121	185.505	146.137	-4.208	1.00	30.91	W
20	ATOM O	2585	OH2	WAT	W	122	168.783	176.131	0.277	1.00	37.59	W
	ATOM O	2586	OH2	WAT	W	123	179.830	187.974	34.894	1.00	39.81	W
	ATOM O	2587	OH2	WAT	W	124	194.391	191.022	26.003	1.00	35.26	W
	ATOM O	2588	OH2	WAT	W	125	175.707	190.116	18.448	1.00	37.47	W
25	ATOM O	2589	OH2	WAT	W	126	172.799	187.052	31.328	1.00	38.58	W
	ATOM O	2590	OH2	WAT	W	127	173.867	181.212	14.618	1.00	28.93	W
	ATOM O	2591	OH2	WAT	W	128	169.850	183.554	9.734	1.00	31.19	W
	ATOM O	2592	OH2	WAT	W	129	201.846	186.034	10.890	1.00	39.65	W
30	ATOM O	2593	OH2	WAT	W	130	192.261	183.101	8.973	1.00	35.20	W
	ATOM O	2594	OH2	WAT	W	131	195.036	155.601	22.286	1.00	43.08	W
	ATOM O	2595	OH2	WAT	W	132	188.136	149.463	-10.689	1.00	31.69	W
	ATOM O	2596	OH2	WAT	W	133	193.611	166.439	22.911	1.00	37.73	W
35	ATOM O	2597	OH2	WAT	W	134	169.159	198.181	-6.371	1.00	34.05	W
	ATOM O	2598	OH2	WAT	W	135	173.141	166.101	3.246	1.00	37.73	W
	ATOM O	2599	OH2	WAT	W	136	196.411	181.887	24.452	1.00	31.18	W
	ATOM O	2600	OH2	WAT	W	137	166.875	190.046	-8.389	1.00	35.44	W
40	ATOM O	2601	OH2	WAT	W	138	168.310	173.985	5.026	1.00	36.83	W
	ATOM O	2602	OH2	WAT	W	139	191.553	162.337	-15.173	1.00	30.34	W
	ATOM O	2603	OH2	WAT	W	140	196.789	179.956	0.077	1.00	34.96	W

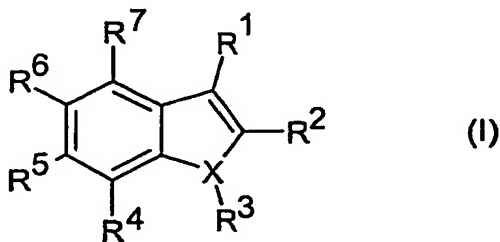
10. Okt. 2003

Claims

1. A crystal of phosphorylated human Aurora-A kinase fragment comprising amino acid residues 122-403 complexed with amino acid residues 1-43 of human TPX2, wherein said crystal diffracts to at least 3 angstrom resolution and has a crystal stability within 5% of its unit cell dimensions.
2. The crystal according to claim 1, having the coordinates as listed in Table B.
3. The crystal according to claim 1 or 2, said crystal belonging to the orthorhombic space group $P2_12_12_1$ and having the unit cell dimensions in angstroms: $a = 59.63 \pm 5\%$, $b = 81.72 \pm 5\%$, $c = 70.38 \pm 5\%$.
4. The crystal according to any one of claims 1 to 3, having a Aurora-A ligand binding site defined by the structure coordinates of Aurora-A amino acids Q127, W128, R126, L159, F157, E170, L169, V206, Y199, H187, R179, L178, V182, Y199, L188, I184, V252, K250, P282, H280 according to Table B.
5. A molecule or molecular complexe comprising at least a part of the ligand binding site defined by structure coordinates of Aurora-A amino acids Q127, W128, R126, L159, F157, E170, L169, V206, Y199, H187, R179, L178, V182, Y199, L188, I184, V252, K250, P282, H280 according to Table B, or a mutant or homologue thereof.
6. A machine-readable data storage medium comprising a data storage material encoded with machine readable data, wherein the data is defined by the structure coordinates of phosphorylated human Aurora-A kinase complexed with amino acid residues 1-43 of human TPX2 according to Table B or a homologue of said complex, wherein said homologue comprises backbone atoms that have a root mean square deviation from the backbone atoms of the complex of not more than 3.0 Å.
7. A binding site in Aurora-A, or a homologue or mutant thereof, for an AR modulator in which a portion of said ligand is in van der Waals contact or hydrogen bonding contact with any portion or all of residues Q127, W128, R126, L159, F157, E170, L169, V206, Y199, H187, R179, L178, V182, Y199, L188, I184, V252, K250, P282, H280 of Aurora-A according to Table B.
8. The binding site according to claim 7, wherein the homologue or mutant has 25%-95% identity to residues Q127, W128, R126, L159, F157, E170, L169, V206, Y199,

H187, R179, L178, V182, Y199, L188, I184, V252, K250, P282, H280 of Aurora-A according to Table B.

9. A method for identifying a compound that modulates Aurora-A kinase activity, the method comprising any combination of steps of :
 - a) modeling test compounds that fit spatially into the Aurora-A binding site as defined by structure coordinates according to Table B;
 - b) using said structure coordinates or binding site as set forth in claim 7 to identify structural and chemical features;
 - c) employing identified structural or chemical features to design or select compounds as potential Aurora-A modulators;
 - d) employing the three-dimensional structural model or the ligand binding site to design or select compounds as potential Aurora-A modulators;
 - e) synthesizing the potential Aurora-A modulators;
 - f) screening the potential Aurora-A modulators in an assay characterized by binding of a test compound to the Aurora-A; and
 - g) modifying or replacing one or more amino acids from Aurora-A selected from the group consisting of Q127, W128, R126, L159, F157, E170, L169, V206, Y199, H187, R179, L178, V182, Y199, L188, I184, V252, K250, P282, H280 of Aurora-A according to Table B.
10. An Aurora-A modulator identified by the method of claim 9.
11. An allosteric inhibitor of Aurora-A, at least a portion of which binds with any portion or all of residues Q127, W128, R126, L159, F157, E170, L169, V206, Y199, H187, R179, L178, V182, Y199, L188, I184, V252, K250, P282, H280 of Aurora-A according to Table B.
12. The allosteric inhibitor of claim 11, wherein binding is van der Waals contact or hydrogen bonding contact.
13. Indole and indene derivatives of formula (I)



wherein

R^1 represents hydrogen, alkylene-NHR⁸, alkylene-OR⁸, or alkylene-SR⁸;

R^2 represents hydrogen, alkylene-NHR⁸, alkylene-OR⁸, or alkylene-SR⁸;

5 R^3 represents hydrogen, alkyl, alkylene-R⁹, alkenylene-R⁹, alkynylene-R⁹, or arylene-R⁹;

R^4 represents hydrogen;

R^5 represents hydrogen, alkyl, OR¹⁰, NHR¹⁰, SR¹⁰, alkylene-R¹⁰, alkenylene-R¹⁰, alkynylene-R¹⁰, or arylene-R¹⁰;

10 R^6 represents hydrogen, alkyl, OR¹⁰, NHR¹⁰, SR¹⁰, alkylene-R¹⁰, alkenylene-R¹⁰, alkynylene-R¹⁰, or arylene-R¹⁰;

R^7 represents hydrogen;

R^8 represents hydrogen, CO-alkyl, (aa)_masp(aa)_n, (aa)_mglu(aa)_n, or (aa)_mcys(aa)_n;

15 R^9 represents NH-alkyl, N(alkyl)₂, N⁺(alkyl)₃, aryl, or heteroaryl;

R^{10} represents hydrogen, aryl, or substituted aryl;

X represents a nitrogen atom or CH;

aa represents an amino acid radical; and

n is zero or an integer of 1 to 10;

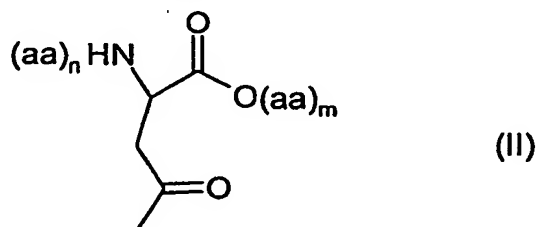
20 m is zero or an integer of 1 to 10,

provided that R^1 and R^2 are not both hydrogen and that R^5 and R^6 are not both hydrogen,

and optical isomers, physiologically acceptable salts and prodrugs thereof.

25 14. The compound according to claim 13, wherein one of residues R^1 and R^2 , preferably R^2 , is hydrogen and the other, preferably R^1 , represents alkylene-NHR⁸.

15. The compound according to claim 13 or 14, wherein R^8 is a radical of the formula (II)



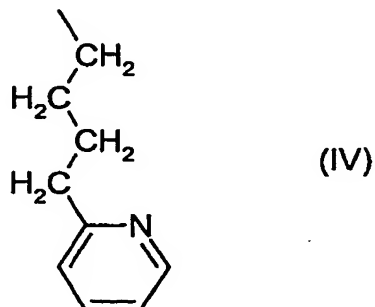
30 wherein

aa represents an amino acid radical;

n is zero or an integer of 1 to 10; and

m is zero or an integer of 1 to 10.

16. The compound according to any one of claims 13 to 15, wherein R^3 is a radical of the formula (IV)



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17. The compound according to any one of claims 13 to 16, wherein R^5 and/or R^6 represent OR^{10} , wherein R^{10} is defined as in claim 13.

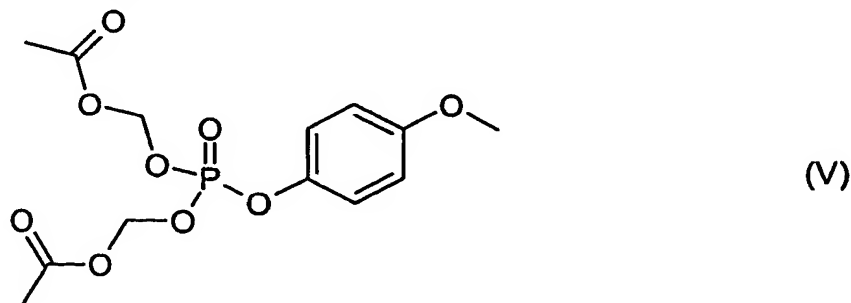
18. The compound according to any one of claims 13 to 17, wherein R^{10} is aryl which may be substituted with 1, 2 or 3 substituents independently selected from the group consisting of hydroxy $-OPO_3H_2$, $-CH_2PO_3H_2$, $-CF_2PO_3H_2$, $-COOH$, $-CH(COOH)_2$, $-OPO_3(R^{11})_2$, $-CH_2OPO_3(R^{11})_2$, $-CF_2OPO_3(R^{11})_2$, $-COOR^{11}$, and $-CH(COOR^{11})_2$, wherein R^{11} is a radical that is cleavable *in vivo*.

15

19. The compound according to claim 18, wherein R^{11} represents alkyl, CH_2OCO -alkyl, and C_2H_4-S-CO -alkyl.

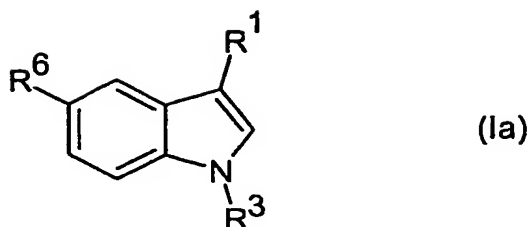
20. The compound according to any one of claims 13 to 19, wherein R^5 and/or R^6 are/is the radical of formula (V)

20



21. The compound according to claim 13, having the formula (Ia)

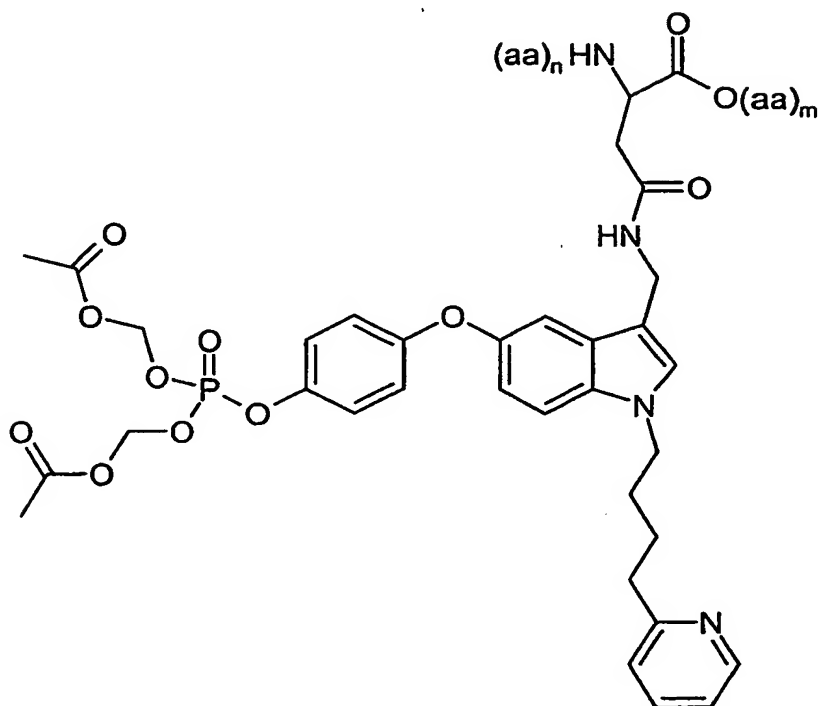
25



wherein

5 R^1 , R^3 and R^6 are defined as in any one of claims 13 to 20.

22. The indole derivative of formula (1)



10 wherein

aa, n and m are defined as in claim 13,

and optical isomers and physiologically acceptable salts thereof.

23. The Aurora-A modulator of claim 10, the allosteric inhibitor of claims 11 or 12, or the
15 indole or indene derivative of any one of claims 13 to 22 for use in therapy.

24. Pharmaceutical composition, comprising at least one Aurora-A modulator of claim
10, at least one allosteric inhibitor of claims 11 or 12, or at least one indole or indene

derivative of any one of claims 13 to 22, optionally in combination with a pharmaceutically acceptable excipient.

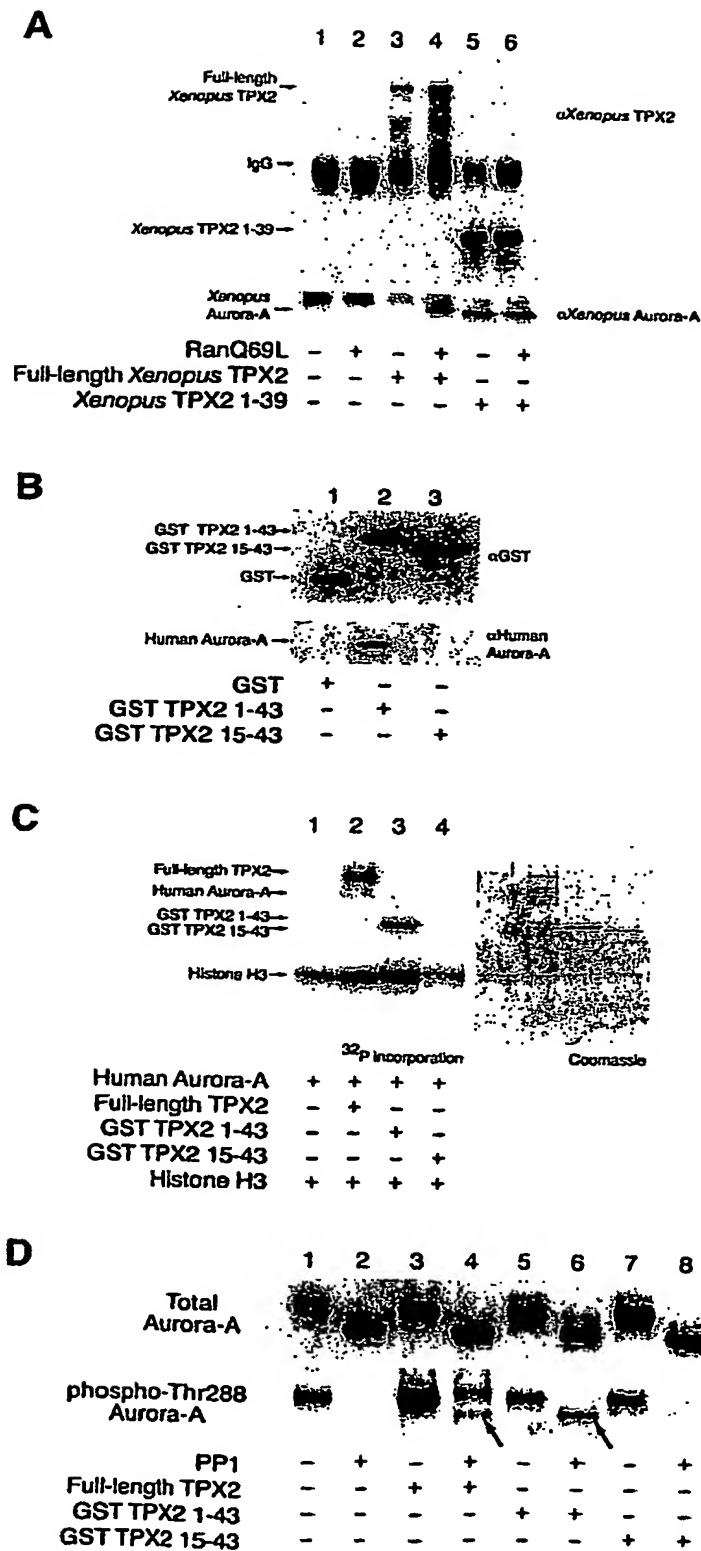
- 5 25. The use of an Aurora-A modulator of claim 10, of an allosteric inhibitor of claims 11 or 12, or of an indole or indene derivative of any one of claims 13 to 22 in the manufacture of a medicament for treating cancer.
26. The use according to claim 25, wherein the cancer is a breast or colon carcinoma.

10. Okt. 2003

The present invention relates to crystals of phosphorylated Aurora-A kinase fragment alone and in complex with a ligand, amino acid residues 1-43 of human TPX2. This invention also
5 relates to methods for designing and selecting ligands, in particular allosteric inhibitors of Aurora-A, that bind to the Aurora-A kinase and their use. Further, the present invention relates to certain indene and indole derivatives. The present invention relates to crystals of phosphorylated Aurora-A kinase alone and in complex with a ligand, amino acid residues 1-43 of human TPX2. This invention also relates to methods for designing and selecting
10 ligands that bind to the Aurora-A kinase and their use. Further, the present invention relates to certain indene and indole derivatives.

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Fig. 1



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Fig. 2

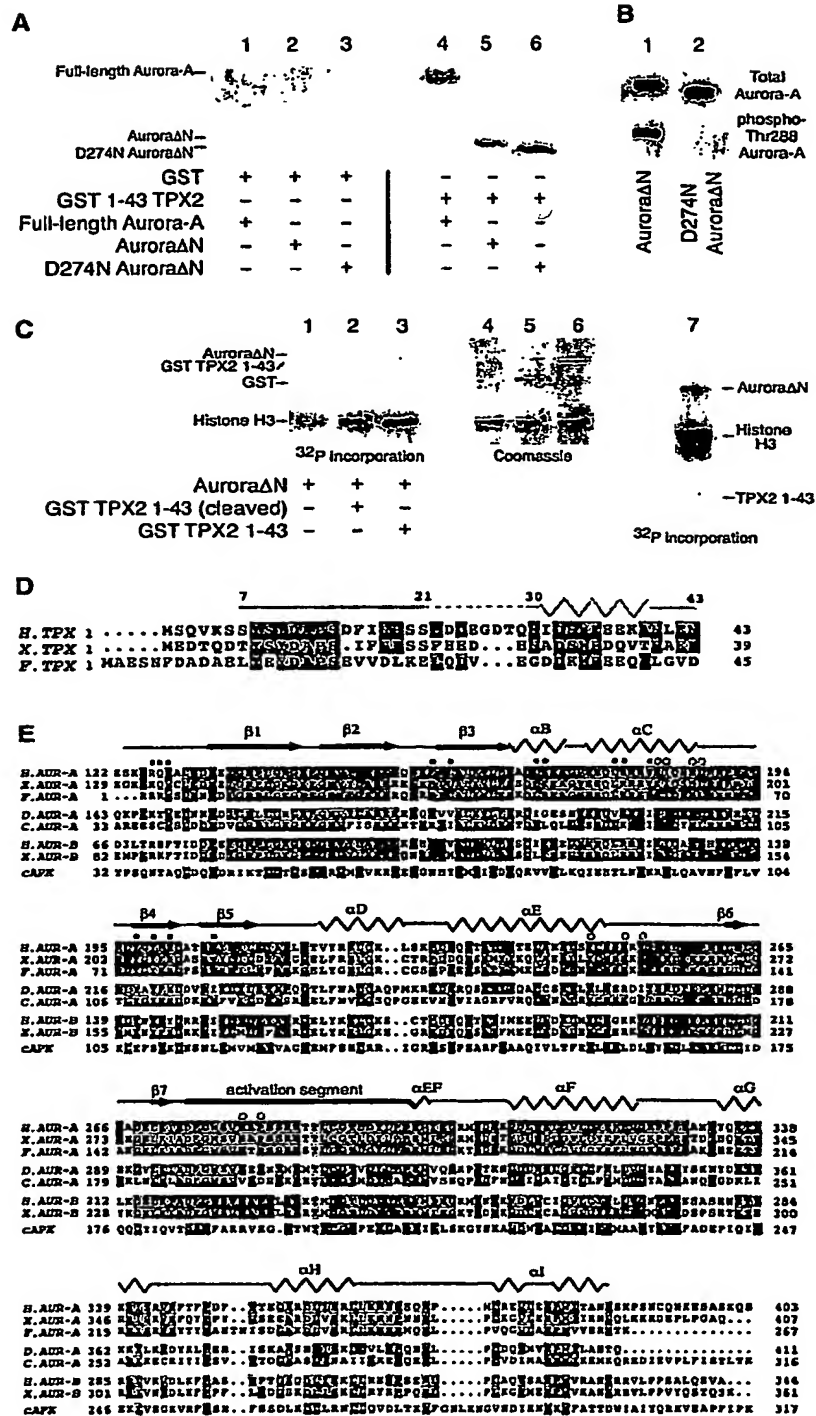


Fig. 3

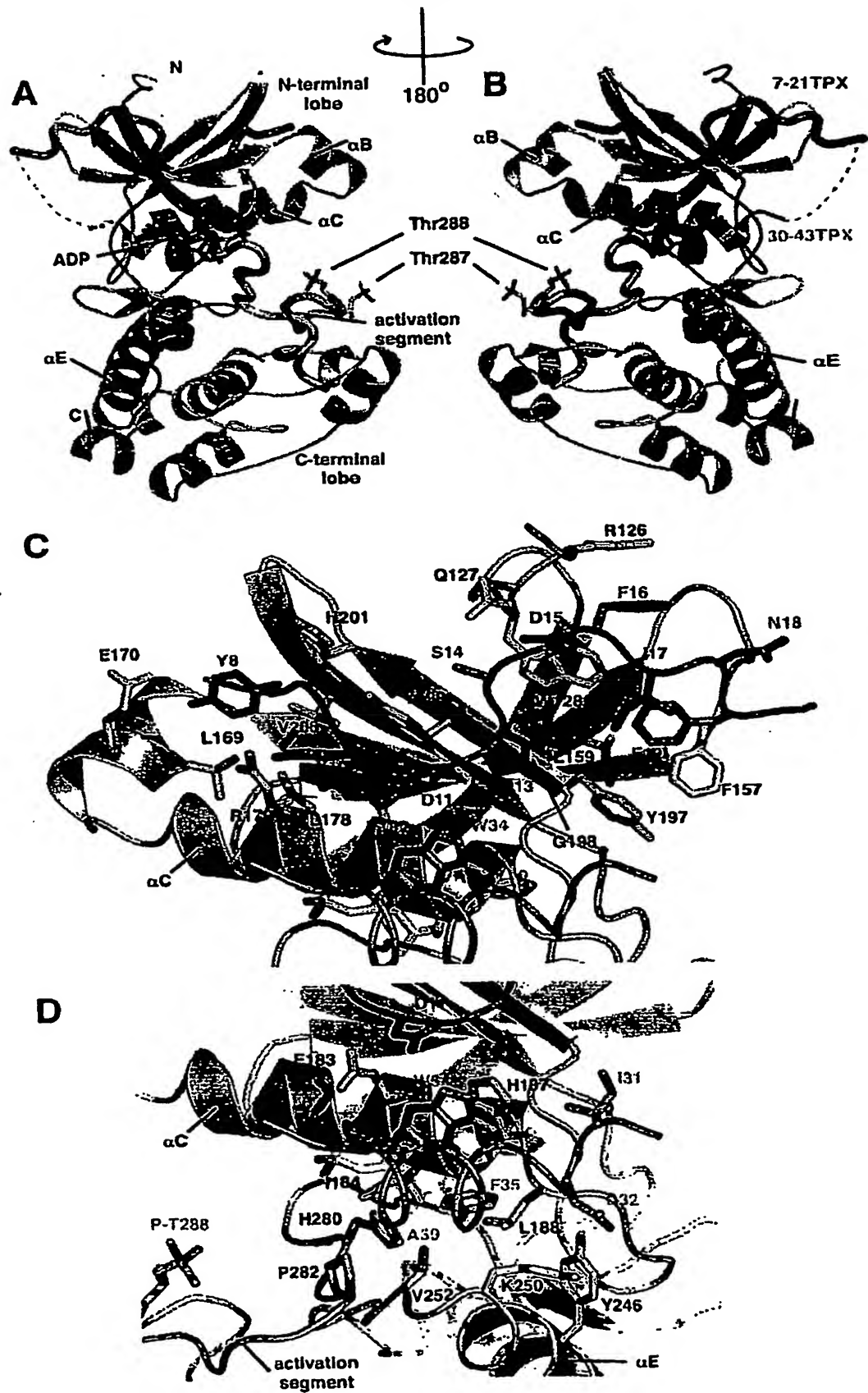
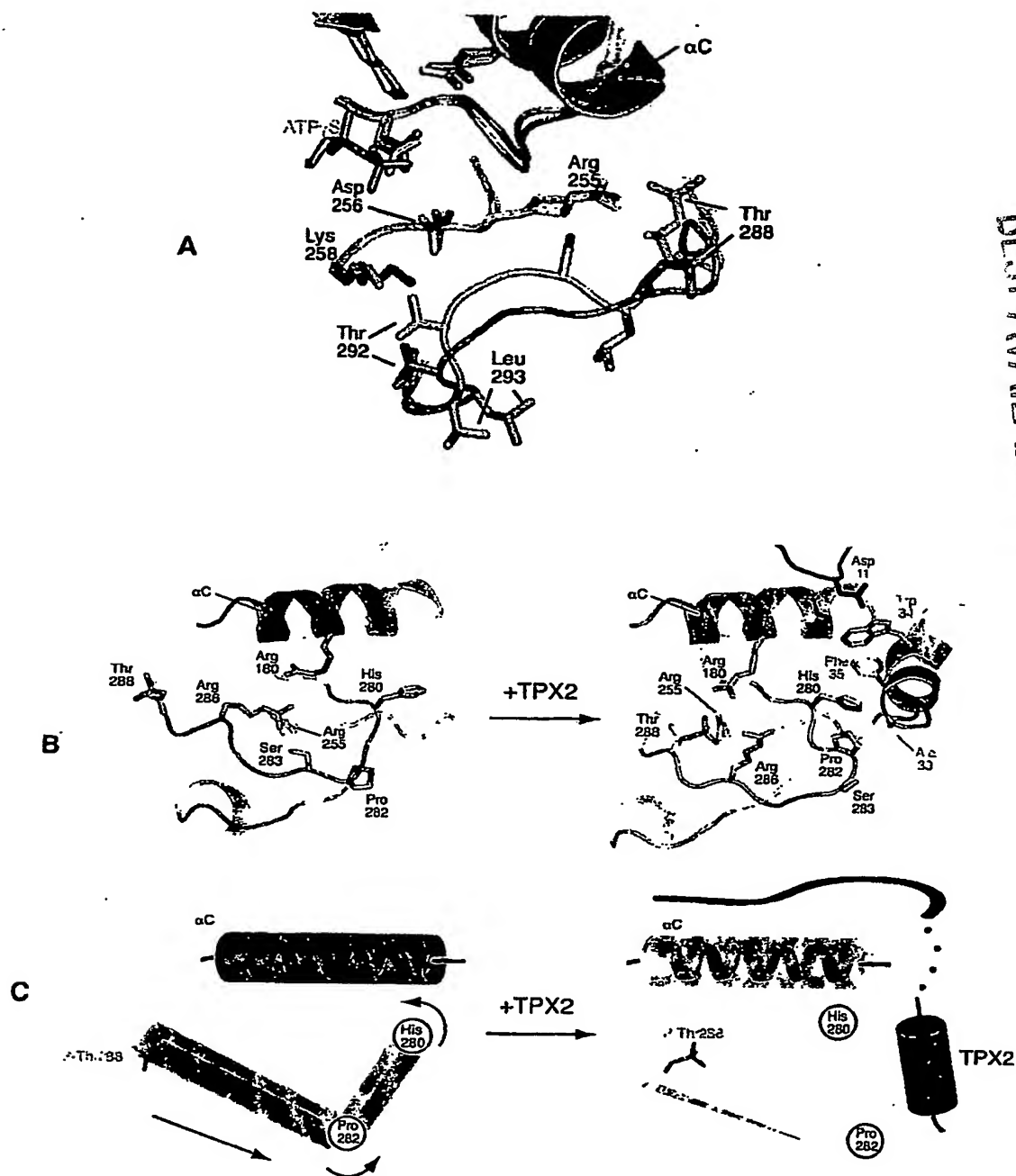


Fig. 4



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